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Thermodynamic Properties of Carbides, Nitrides, and Other Selected Substances

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UNIT OF MEASURE ABBREVIATIONS USED IN THIS BULLETIN

atm	atmosphere (1 atm = 101,325 pascals)
cal	thermochemical calorie (1 cal = 4.1840 joules)
cal/mol	calorie per mole
cal/mol•K	calorie per mole per kelvin
K	kelvin, the unit of thermodynamic temperature
kcal/mol	kilocalorie per mole
mol	mole, gram formula weight or molar mass

OTHER ABBREVIATIONS AND SYMBOLS USED IN THIS BULLETIN

Cp	heat capacity at constant pressure
F	Faraday constant, 23,060.9 cal/V - equivalent
$(G - H_{298})/T$	Gibbs energy function, $[(H - H_{298}/T] - S$
$H - H_{298}$	enthalpy increment between T and 298.15 K
ln	natural logarithm, base e = 2.7183
log K	logarithm (base 10) of the equilibrium constant (log Kf = equilibrium constant of formation)
P	pressure in atmospheres
R	gas constant, 1.98719 cal/mol•K
S	entropy
T	thermodynamic temperature in kelvins
°	standard state
ΔG	Gibbs energy change (ΔGf = Gibbs energy of formation)
ΔH	enthalpy change (ΔHf = enthalpy of formation)

THERMODYNAMIC PROPERTIES OF CARBIDES, NITRIDES, AND OTHER SELECTED SUBSTANCES

By L. B. Pankratz[1]

ABSTRACT

Thermodynamic data on carbides, nitrides, and other selected substances were reviewed, evaluated, and compiled at the U.S. Bureau of Mines Albany Research Center. Values for Cp°, S°, H° - H°_{298}, -(G° - H°_{298})/T, ΔHf°, ΔGf, and log Kf are given in tabular form. Cp°, H° - H°_{298}, ΔHf°, and ΔGf° are also expressed algebraically.

INTRODUCTION

This compilation is the fourth and final in a series revising and expanding U.S. Bureau of Mines (USBM) Bulletin 605, "Thermodynamic Properties of 65 Elements—Their Oxides, Halides, Carbides, and Nitrides," by C. E. Wicks and F. E. Block (532),[2] published in 1963. The first volume in this series, USBM Bulletin 672, "Thermodynamic Properties of Elements and Oxides," by L. B. Pankratz (383), was published in 1982. The second, Bulletin 674, "Thermodynamic Properties of Halides," also by L. B. Pankratz (384), was published in 1984. The third, Bulletin 689, "Thermodynamic Properties of Sulfides," by L. B. Pankratz, A. D. Mah, and S. W. Watson (388), was published in 1987. These three volumes along with the current compilation present thermodynamic data for more than 2,300 substances. They are part of the USBM's continuing effort to provide information for use as guidelines in mineral technology advancement, pollution control, and energy economy.

The values of heat capacities (Cp°), high-temperature relative enthalpies (H° - H°_{298}); enthalpies of formation (ΔHf°), and Gibbs energies of formation (ΔGf°) are given in both tabular and equation forms. The tables also include entropies (S°), Gibbs energy functions [-(G° - H°_{298})/T], and logarithms (base 10) of the equilibrium constants (log Kf). For substances containing sulfur, selenium, and tellurium, the values for ΔH, ΔG, and log K were calculated using S_2(g), Se_2(g), and Te_2(g); therefore, the symbols ΔHf, ΔGf, and log Kf have been replaced with ΔHr, ΔGr, and log Kr.

Where possible, all phases of a substance are presented in a single table. Temperatures of transformation and thermodynamic properties at these temperatures are included in the table. Immediately below the table, the natures of transformations are given along with their associated enthalpies.

Bulletin 672 contains a section, "Process Applications," which gives a short statement of some fundamental ideas of thermodynamics and includes several examples of their use. These examples illustrate several alternative methods of calculation using both the tabulated values and the equations. Comparisons are also made on the basis of ease of calculation and accuracy of results.

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[2] Underlined numbers in parentheses refer to items in the list of references at the end of this bulletin.

METHODS AND CONVENTIONS

The values in this compilation are the result of a review and critical evaluation of relevant thermodynamic data through June 1985, although some data published later have been included. Data for the elements are from Bulletin 672. Many of the data for the actinide compounds are from the International Atomic Energy Agency series on "The Chemical Thermodynamics of Actinide Elements and Compounds" (187). The "JANAF Thermochemical Tables" supplements by M. W. Chase and his coworkers (80-83) were an invaluable source of recent, critically evaluated data. Specific references are made to these publications where they are used.

The selected experimental data were fit with a polynomial in terms of temperature by using a modified form of the computer program described by Justice (225). This program, along with a plot of $(H° - H°_{298})/(T - 298.15)$, which must take the value of Cp° at 298.15 K, was used to merge high-temperature data smoothly with low-temperature heat capacity data. The resulting polynomial was then used in a subroutine of the program to calculate standard heat capacities, entropies, Gibbs energy of formation, and the logarithm of the equilibrium constant of formation.

Tabular values of relative enthalpies are represented by algebraic equations in the form recommended by Maier and Kelley (321). This form was fit to the data by Kelley's method (243). Since the equations consist of no more than four terms, they give less precise values than the tabular values. However, they do furnish a convenient means of representation. These equations are given below each table. A separate equation is given whenever a transformation occurs. In some cases two equations are used to represent a single phase with an extended temperature range, since a single equation would give unacceptable errors.

The equations for standard heat capacity, enthalpy of formation, and Gibbs energy of formation are also given below the tables. Since these equations were derived using the equations for standard relative enthalpies, they too give less precise values than the tabular values. Examples in the "Process Applications" section of Bulletin 672 show the methods of derivation.

Tabulated values and the equations are for the substances in their standard states (indicated by the superscript °). Standard states for the pure condensed substances are the most stable form at 1 atm pressure at the specified temperature. For vitreous and metastable substances, the superscript refers to the pure substance. For gases, the standard state is the pure substance at unit fugacity.

Sources of data used in this compilation are given in the references section, which is not meant to be exhaustive. For simplicity, additional sources reviewed or considered less reliable were not included. Estimates were used where the necessary data were lacking. Estimated and extrapolated values are indicated in the tables with an asterisk (1) and a note immediately below the table. An asterisk and a note are also used to indicate decomposition, metastable phases, and irreversible transformations.

The common practice of tabulating five- and sometimes six-digit values has been followed. For example, enthalpy values are given to the nearest calorie. The number of digits given is not intended to reflect the accuracy of the experimental values used. It is an effort to produce internal consistency in the tabulated values.

THERMODYNAMIC DATA FOR CARBIDES, NITRIDES, AND OTHER SELECTED SUBSTANCES

In the following pages, thermodynamic values are given in both tabular and equation forms. The tables have the base temperature 298.15 K and are not extended much above the temperature of the available data. Except in tables or equations, the base temperature is usually abbreviated as 298 K. To avoid confusion, the standard state at 298.15 K is indicated in each table heading and in the chemical formation equation. The symbols c, l, g, and vit refer respectively to crystal, liquid, gas, and vitreous phases. Also, the Greek letters α, β, γ, δ, and ϵ are used to denote different crystalline forms. In a few instances, Greek letters also denote substances above and below a second-order transformation. Again, to avoid confusion, where substances have the same formula but different standard states, the standard state is explicitly given in the table heading, for example, AlN(g) or AlO(OH) (diaspore) and AlO (OH) (boehmite).

Many of the experimental measurements of thermodynamic properties used in this compilation were obtained using the International Practical Temperature Scale of 1948 (IPTS-48). This temperature scale has been superseded by IPTS-68 (95) and the amended edition of 1975 (96). These scales differ by as much as 2.6 K (at 2,000 K), but no attempt has been made, except as specifically noted, to convert earlier measurements to IPTS-68 since the errors involved are less than experimental errors.

The tables are arranged in alphabetical order by chemical symbols. For convenience, the chemical symbol of the pertinent element has been included in pagination.

$Ag_2CO_3(c)$
Silver Carbonate
[Formation: $2Ag(c) + C(c) + 1.5O_2(g) = Ag_2CO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	26.830	40.000	40.000	0	-120.880	-104.416	76.538
300	26.840	40.166	40.003	.049	-120.876	-104.314	75.992
350	28.083	44.390	40.333	1.420	-120.756	-101.564	63.419
400	29.314	48.230	41.080	2.860	-120.598	-98.831	53.998
450	30.473	51.740	42.073	4.350	-120.422	-96.121	46.682
500	31.501	55.000	43.200	5.900	-120.218	-93.429	40.837

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp° = 19.570 + 24.360\times10^{-3}T$

$H°-H°_{298} = 19.570\times10^{-3}T + 12.180\times10^{-6}T^2 - 6.918$

Formation equations (kcal/mol):

298.15-500 K: $\Delta Hf° = -119.417 - 5.337\times10^{-3}T + 8.823\times10^{-6}T^2 - 195.700T^{-1}$

$\Delta Gf° = -119.417 + 5.337\times10^{-3}T\ln T - 8.823\times10^{-6}T^2 - 97.850T^{-1} + 23.635\times10^{-3}T$

Source: Data from Chang (74).

$Ag_2CrO_4(c)$
Silver Chromate
[Formation: $2Ag(c) + Cr(c) + 2O_2(g) = Ag_2CrO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	34.000	52.000	52.000	0	-174.890	-153.423	112.461
300*	34.050	52.210	52.010	.060	-174.888	-153.293	111.672
311.5	34.308	53.496	52.041	.453	-174.863	-152.465	106.969
350	35.170	57.550	52.436	1.790	-174.819	-149.705	93.479
400	36.060	62.310	53.360	3.580	-174.593	-146.133	79.842
450	36.860	66.600	54.600	5.400	-174.424	-142.585	69.248
500	37.590	70.520	56.000	7.260	-174.243	-139.057	60.781
550	38.260	74.140	57.485	9.160	-174.047	-135.543	53.859
600	38.820	77.490	59.007	11.090	-173.851	-132.047	48.097

*Data above 298 K estimated.

Phase change: 311.5 K, second-order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 32.911 + 10.926\text{x}10^{-3}T - 1.928\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 32.911\text{x}10^{-3}T + 5.463\text{x}10^{-6}T^{2} + 1.928\text{x}10^{2}T^{-1} - 10.945$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -177.560 + 10.715\text{x}10^{-3}T - 11.446\text{x}10^{-6}T^{2} + 146.800T^{-1}$
$\Delta Gf° = -177.560 - 10.715\text{x}10^{-3}T\ln T + 11.446\text{x}10^{-6}T^{2} + 73.400T^{-1} + 137.765\text{x}10^{-3}T$
311.5-600 K: $\Delta Hf° = -176.562 + 3.548\text{x}10^{-3}T + 0.830\text{x}10^{-6}T^{2} + 160.400T^{-1}$
$\Delta Gf° = -176.562 - 3.548\text{x}10^{-3}T\ln T - 0.830\text{x}10^{-6}T^{2} + 80.200T^{-1} + 97.168\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Low-temperature heat capacities and entropy at 298 K from Smith (466). High-temperature data estimated.

$AgNO_3(c,l)$
Silver Nitrate
[Formation: $Ag(c) + 0.5N_2(g) + 1.5O_2(g) = AgNO_3(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	22.240	33.680	33.680	0	-29.730	-8.000	5.864
300	22.300	33.820	33.687	.040	-29.727	-7.867	5.731
400	25.920	40.740	34.615	2.450	-29.342	-.635	.347
433	27.120	42.840	35.146	3.330	-29.140	1.732	-.874
433	29.580	44.150	35.146	3.900	-28.570	1.732	-.874
483	28.410	47.330	36.251	5.350	-28.158	5.207	-2.356
483	31.000	53.330	36.251	8.250	-25.258	5.207	-2.356
500	31.000	54.400	36.840	8.780	-25.084	6.281	-2.745
600	31.000	60.050	40.250	11.880	-24.108	12.464	-4.540

Phase changes: 433 K, α - β transition point of $AgNO_3$; ΔH° = 0.570 kcal/mol.
483 K, melting point of $AgNO_3$; ΔH° = 2.900 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-433 K: $Cp° = 10.925 + 37.036\times10^{-3}T + 0.296\times10^{5}T^{-2}$
$H° - H°_{298} = 10.925\times10^{-3}T + 18.518\times10^{-6}T^{2} - 0.296\times10^{2}T^{-1} - 4.804$
433-483 K: $Cp° = 39.719 - 23.406\times10^{-3}T$
$H° - H°_{298} = 39.719\times10^{-3}T - 11.703\times10^{-6}T^{2} - 11.104$
483-600 K: $Cp° = 31.000$
$H° - H°_{298} = 31.000\times10^{-3}T - 6.723$

Formation equations (kcal/mol):

298.15-433 K: $\Delta Hf° = -28.443 - 8.450\times10^{-3}T + 16.551\times10^{-6}T^{2} - 71.250T^{-1}$
$\Delta Gf° = -28.443 + 8.450\times10^{-3}T\ln T - 16.551\times10^{-6}T^{2} - 35.625T^{-1} + 25.753\times10^{-3}T$
433-483 K: $\Delta Hf° = -34.743 + 20.344\times10^{-3}T - 13.670\times10^{-6}T^{2} - 41.650T^{-1}$
$\Delta Gf° = -34.743 - 20.344\times10^{-3}T\ln T + 13.670\times10^{-6}T^{2} - 20.825T^{-1} + 201.939\times10^{-3}T$
483-600 K: $\Delta Hf° = -30.362 + 11.625\times10^{-3}T - 1.967\times10^{-6}T^{2} - 41.650T^{-1}$
$\Delta Gf° = -30.362 - 11.625\times10^{-3}T\ln T + 1.967\times10^{-6}T^{2} - 20.825T^{-1} + 144.637\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Low-temperature heat capacities and entropy at 298 K from Smith (465). High-temperature data based on Janz (216), Reinsborough (419), Kelley (243), and Kleppa (274).

AgO(g)
Silver Monoxide (ideal gas)
[Formation: $Ag(c,l) + 0.5O_2(g) = AgO(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.410	58.685	58.685	0	75.000	67.841	-49.728
300	8.420	58.738	58.685	.016	74.998	67.797	-49.389
400	8.660	61.200	59.020	.872	74.888	65.412	-35.739
500	8.780	63.147	59.657	1.745	74.772	63.056	-27.562
600	8.860	64.754	60.377	2.626	74.641	60.726	-22.119
700	8.910	66.123	61.102	3.515	74.490	58.420	-18.239
800	8.950	67.316	61.806	4.408	74.315	56.134	-15.335
900	8.980	68.371	62.478	5.304	74.119	53.872	-13.082
1000	9.010	69.320	63.116	6.204	73.905	51.633	-11.284
1100	9.040	70.181	63.720	7.107	73.668	49.418	-9.818
1200	9.060	70.969	64.292	8.012	73.407	47.224	-8.601
1235.08	9.071	71.230	64.486	8.330	73.309	46.464	-8.222
1235.08	9.071	71.230	64.486	8.330	70.609	46.464	-8.222
1300	9.090	71.696	64.834	8.920	70.401	45.200	-7.599
1400	9.110	72.369	65.348	9.830	70.080	43.276	-6.756
1500	9.140	73.000	65.838	10.743	69.758	41.371	-6.028
1600	9.160	73.590	66.304	11.657	69.433	39.488	-5.394
1700	9.190	74.146	66.750	12.574	69.109	37.627	-4.837
1800	9.210	74.672	67.175	13.494	68.785	35.784	-4.345
1900	9.230	75.170	67.583	14.416	68.460	33.961	-3.906
2000	9.260	75.644	67.973	15.341	68.136	32.154	-3.514

Phase change: 1235.08 K, melting point of Ag; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.865 + 0.196\times10^{-3}T - 0.457\times10^{5}T^{-2}$
$H°-H°_{298} = 8.865\times10^{-3}T + 0.098\times10^{-6}T^{2} + 0.457\times10^{2}T^{-1} - 2.805$

Formation equations (kcal/mol):

298.15-1235.08 K: $\Delta Hf° = 74.950 - 0.022\times10^{-3}T - 1.072\times10^{-6}T^{2} + 45.300T^{-1}$
$\Delta Gf° = 74.950 + 0.022\times10^{-3}T\ln T + 1.072\times10^{-6}T^{2} + 22.650T^{-1} - 24.544\times10^{-3}T$
1235.08-2000 K: $\Delta Hf° = 74.237 - 2.750\times10^{-3}T - 0.153\times10^{-6}T^{2} + 23.100T^{-1}$
$\Delta Gf° = 74.237 + 2.750\times10^{-3}T\ln T + 0.153\times10^{-6}T^{2} + 11.550T^{-1} - 42.246\times10^{-3}T$

Source: Data from Pedley (396).

Ag_2SO_4(c,l)
Silver Sulfate
[Reaction: $2Ag(c) + 0.5S_2(g) + 2O_2(g) = Ag_2SO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	31.523	48.020	48.020	0	-186.395	-157.301	115.303
300	31.606	48.215	48.022	.058	-186.392	-157.119	114.460
400	35.312	57.846	49.309	3.415	-186.078	-147.403	80.536
500	38.217	66.046	51.856	7.095	-185.520	-137.794	60.229
600	40.833	73.247	54.832	11.049	-184.770	-128.312	46.737
698.6	43.309	79.645	57.890	15.198	-183.862	-119.104	37.260
698.6	43.732	85.229	57.890	19.099	-179.961	-119.104	37.260
700	43.754	85.316	57.945	19.160	-179.947	-118.982	37.147
800	45.348	91.263	61.744	23.615	-178.859	-110.349	30.145
900	46.941	96.696	65.330	28.229	-177.683	-101.858	24.734
926	47.355	98.039	66.230	29.455	-177.362	-99.672	23.524
926	35.000	102.963	66.230	34.015	-172.802	-99.672	23.524
1000	35.000	105.653	69.048	36.605	-172.807	-93.826	20.505
1025	35.000	106.518	69.952	37.480	-172.818	-91.852	19.584

Phase changes: 698.6 K, α - β transition point of Ag_2SO_4; ΔH° = 3.901 kcal/mol.
926 K, melting point of Ag_2SO_4; ΔH° = 4.560 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-698.6 K: $Cp° = 28.185 + 22.478\times10^{-3}T - 2.993\times10^{5}T^{-2}$
$H°-H°_{298} = 28.185\times10^{-3}T + 11.239\times10^{-6}T^{2} + 2.993\times10^{2}T^{-1} - 10.406$
698.6-926 K: $Cp° = 32.056 + 16.394\times10^{-3}T + 1.096\times10^{5}T^{-2}$
$H°-H°_{298} = 32.056\times10^{-3}T + 8.197\times10^{-6}T^{2} - 1.096\times10^{2}T^{-1} - 7.139$
926-1025 K: $Cp° = 35.000$
$H°-H°_{298} = 35.000\times10^{-3}T + 1.605$

Reaction equations (kcal/mol):

298.15-698.6 K: $\Delta Hr° = -187.567 - 0.991\times10^{-3}T + 8.237\times10^{-6}T^{2} + 219.150T^{-1}$
$\Delta Gr° = -187.567 + 0.991\times10^{-3}T\ln T - 8.237\times10^{-6}T^{2} + 109.575T^{-1} + 97.093\times10^{-3}T$
698.6-926 K: $\Delta Hr° = -184.300 + 2.881\times10^{-3}T + 5.195\times10^{-6}T^{2} - 189.750T^{-1}$
$\Delta Gr° = -184.300 - 2.881\times10^{-3}T\ln T - 5.195\times10^{-6}T^{2} - 94.875T^{-1} + 116.063\times10^{-3}T$
926-1025 K: $\Delta Hr° = -175.556 + 5.825\times10^{-3}T - 3.002\times10^{-6}T^{2} - 80.150T^{-1}$
$\Delta Gr° = -175.556 - 5.825\times10^{-3}T\ln T + 3.002\times10^{-6}T^{2} - 40.075T^{-1} + 119.075\times10^{-3}T$

Source: Data from DeKock (113).

$Ag_3Sb(c)$
Trisilver Antimonide
[Formation: $3Ag(c) + Sb(c) = Ag_3Sb(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	24.300	41.000	41.000	0	-5.500	-5.384	3.946
300	24.330	41.150	41.017	.040	-5.504	-5.386	3.924
400	25.930	48.370	41.970	2.560	-5.432	-5.350	2.923
500	27.530	54.330	43.870	5.230	-5.258	-5.351	2.339
600	29.130	59.490	46.057	8.060	-4.973	-5.396	1.965
700	30.730	64.100	48.300	11.060	-4.585	-5.485	1.713
800	32.330	68.310	50.547	14.210	-4.125	-5.655	1.545

*Data at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 19.530 + 16.000 \times 10^{-3}T$
$H° - H°_{298} = 19.530 \times 10^{-3}T + 8.000 \times 10^{-6}T^2 - 6.534$

Formation equations (kcal/mol):

298.15-800 K: $\Delta Hf° = -5.748 - 1.374 \times 10^{-3}T + 4.074 \times 10^{-6}T^2 + 88.200T^{-1}$
$\Delta Gf° = -5.748 + 1.374 \times 10^{-3}T\ln T - 4.074 \times 10^{-6}T^2 + 44.100T^{-1} - 5.887 \times 10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K are those estimated by Kubaschewski (290). Heat capacity at 298 K estimated. High-temperature data from Kelley (243).

$Ag_2Se(c)$
Disilver Selenide
[Reaction: $2Ag(c) + 0.5Se_2(g) = Ag_2Se(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	19.480	35.890	35.890	0	-27.050	-23.010	16.867
300	19.510	36.010	35.893	.035	-27.046	-22.985	16.744
400	20.820	41.810	36.673	2.055	-26.747	-21.675	11.843
406	20.900	42.120	36.751	2.180	-26.727	-21.600	11.627
406	20.160	46.640	36.751	4.015	-24.892	-21.600	11.627
500	20.380	50.860	39.020	5.920	-24.632	-20.865	9.120
600	20.600	54.590	41.308	7.969	-24.359	-20.132	7.333
700*	20.830	57.790	43.447	10.040	-24.095	-19.453	6.074
800	21.060	60.580	45.413	12.134	-23.841	-18.803	5.137
900	21.280	63.080	47.246	14.251	-23.596	-18.198	4.419
1000	21.510	65.330	48.938	16.392	-23.357	-17.606	3.848

*Data above 630 K extrapolated.

Phase change: 406 K, α - β transition point of Ag_2Se; ΔH° = 1.835 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-406 K: $Cp° = 18.223 + 8.016x10^{-3}T - 1.007x10^{5}T^{-2}$
$H°- H°_{298} = 18.223x10^{-3}T + 4.008x10^{-6}T^{2} + 1.007x10^{2}T^{-1} - 6.127$
406-1000 K: $Cp° = 19.221 + 2.292x10^{-3}T + 0.015x10^{5}T^{-2}$
$H°- H°_{298} = 19.221x10^{-3}T + 1.146x10^{-6}T^{2} - 0.015x10^{2}T^{-1} - 3.974$

Reaction equations (kcal/mol):

298.15-406 K: $ΔHr° = -28.343 + 2.347x10^{-3}T + 2.331x10^{-6}T^{2} + 115.150T^{-1}$
$ΔGr° = -28.343 - 2.347x10^{-3}TlnT - 2.331x10^{-6}T^{2} + 57.575T^{-1} + 31.307x10^{-3}T$
406-1000 K: $ΔHr° = -26.190 + 3.345x10^{-3}T - 0.530x10^{-6}T^{2} + 12.950T^{-1}$
$ΔGr° = -26.190 - 3.345x10^{-3}TlnT + 0.530x10^{-6}T^{2} + 6.475T^{-1} + 31.146x10^{-3}T$

Sources: Enthalpy of transition at 406 K from Shukla (456). All other data from Mills (332) who extrapolated above 630 K.

$Ag_2Te(c)$
Disilver Telluride
[Reaction: $2Ag(c) + 0.5Te_2(g) = Ag_2Te(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15	20.320	36.700	36.700	0	-27.765	-23.419	17.167
300	20.360	36.840	36.707	.040	-27.755	-23.394	17.042
400	22.670	43.000	37.528	2.189	-27.270	-22.008	12.024
421	23.180	44.180	37.833	2.671	-27.141	-21.736	11.283
421	20.840	47.920	37.833	4.248	-25.564	-21.736	11.283
500	20.310	51.460	39.718	5.871	-25.282	-21.044	9.198
600	20.080	55.130	41.990	7.884	-24.995	-20.219	7.365
700	20.080	58.220	44.089	9.892	-24.754	-19.440	6.069
800	20.080	60.900	46.025	11.900	-24.555	-18.696	5.107

Phase change: 421 K, α - β transition point of Ag_2Te; ΔH° = 1.577 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-421 K: $Cp^\circ = 12.181 + 25.582\times10^{-3}T + 0.455\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 12.181\times10^{-3}T + 12.791\times10^{-6}T^2 - 0.455\times10^{2}T^{-1} - 4.616$
421-800 K: $Cp^\circ = 20.940 - 1.228\times10^{-3}T$
$H^\circ - H^\circ_{298} = 20.940\times10^{-3}T - 0.614\times10^{-6}T^2 - 4.459$

Reaction equations (kcal/mol):

298.15-421 K: $\Delta Hr^\circ = -27.874 - 2.662\times10^{-3}T + 10.659\times10^{-6}T^2 - 13.200T^{-1}$
$\Delta Gr^\circ = -27.874 + 2.662\times10^{-3}T\ln T - 10.659\times10^{-6}T^2 - 6.600T^{-1} + 3.024\times10^{-3}T$
421-800 K: $\Delta Hr^\circ = -27.717 + 6.097\times10^{-3}T - 2.747\times10^{-6}T^2 + 32.300T^{-1}$
$\Delta Gr^\circ = -27.717 - 6.097\times10^{-3}T\ln T + 2.747\times10^{-6}T^2 + 16.150T^{-1} + 49.806\times10^{-3}T$

Source: Data from Mills (332).

AlB_2(c)
Aluminum Diboride
[Formation: Al(c,l) + 2B(β) = AlB_2(c)]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	10.431	8.300	8.300	0	-16.000	-15.614	11.445
300	10.491	8.365	8.300	.020	-16.001	-15.609	11.371
400	12.814	11.735	8.742	1.197	-16.056	-15.474	8.454
500	14.257	14.758	9.650	2.554	-16.137	-15.315	6.694
600	15.354	17.458	10.730	4.037	-16.255	-15.144	5.516
700	16.287	19.897	11.868	5.620	-16.390	-14.945	4.666
800	17.133	22.127	13.013	7.291	-16.530	-14.728	4.023
900	17.929	24.192	14.142	9.045	-16.674	-14.494	3.520
933.61	18.186	24.854	14.516	9.652	-16.723	-14.412	3.374
933.61	18.186	24.854	14.516	9.652	-19.303	-14.412	3.374
1000	18.693	26.120	15.244	10.876	-19.369	-14.060	3.073
1100	19.437	27.937	16.316	12.783	-19.429	-13.539	2.690
1200	20.166	29.660	17.358	14.763	-19.446	-12.998	2.367
1300	20.886	31.302	18.367	16.816	-19.420	-12.455	2.094

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1300 K:
$$Cp° = 12.180 + 6.850\times10^{-3}T - 3.370\times10^{5}T^{-2}$$
$$H°-H°_{298} = 12.180\times10^{-3}T + 3.425\times10^{-6}T^{2} + 3.370\times10^{2}T^{-1} - 5.066$$

Formation equations (kcal/mol):

298.15-933.61 K:
$$\Delta Hf° = -15.177 - 1.858\times10^{-3}T + 0.314\times10^{-6}T^{2} - 88.600T^{-1}$$
$$\Delta Gf° = -15.177 + 1.858\times10^{-3}T\ln T - 0.314\times10^{-6}T^{2} - 44.300T^{-1} - 11.459\times10^{-3}T$$

933.61-1300 K:
$$\Delta Hf° = -16.444 - 4.856\times10^{-3}T + 2.041\times10^{-6}T^{2} - 106.000T^{-1}$$
$$\Delta Gf° = -16.444 + 4.856\times10^{-3}T\ln T - 2.041\times10^{-6}T^{2} - 53.000T^{-1} - 28.983\times10^{-3}T$$

Source: Data from Barin (23) who estimated all except enthalpy of formation at 298 K.

$AlB_{12}(c)$
Aluminum Dodecaboride
[Formation: Al(c,l) + 12B(β,l) = $AlB_{12}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	35.750	28.400	28.400	0	-48.000	-49.402	36.213
300	36.083	28.622	28.400	.067	-48.004	-49.399	35.987
400	48.750	40.942	29.995	4.379	-48.094	-49.875	27.250
500	56.090	52.666	33.372	9.647	-48.334	-50.266	21.971
600	61.333	63.376	37.494	15.529	-48.803	-50.643	18.446
700	65.587	73.159	41.900	21.881	-49.349	-50.888	15.888
800	69.313	82.165	46.379	28.629	-49.872	-51.060	13.949
900	72.732	90.528	50.825	35.733	-50.356	-51.179	12.428
933.61	73.817	93.215	52.303	38.196	-50.502	-51.207	11.987
933.61	73.817	93.215	52.303	38.196	-53.082	-51.207	11.987
1000	75.960	98.360	55.191	43.169	-53.326	-51.057	11.158
1100	79.064	105.746	59.454	50.921	-53.581	-50.890	10.111
1200	82.083	112.755	63.606	58.979	-53.710	-50.616	9.218
1300	85.043	119.442	67.645	67.336	-53.720	-50.317	8.459
1400	87.959	125.852	71.576	75.986	-53.605	-50.062	7.815
1500	90.843	132.019	75.401	84.927	-53.379	-49.769	7.251
1600	93.703	137.973	79.127	94.154	-53.047	-49.682	6.786
1700	96.544	143.739	82.758	103.667	-52.597	-49.474	6.360
1800	99.370	149.338	86.304	113.462	-52.033	-49.167	5.970
1900	102.185	154.786	89.765	123.540	-51.354	-49.007	5.637
2000	104.990	160.098	93.149	133.899	-50.562	-49.058	5.361
2100	107.787	165.289	96.461	144.538	-49.658	-48.879	5.087
2200	110.579	170.367	99.705	155.456	-48.643	-48.982	4.866
2300	113.364	175.344	102.886	166.653	-47.517	-48.881	4.645
2350	114.755	177.797	104.454	172.356	-46.909	-49.122	4.568
2350	114.755	177.797	104.454	172.356	-190.909	-49.122	4.568
2400	116.146	180.228	106.008	178.129	-190.016	-46.002	4.189
2473	118.174	183.738	108.250	186.682	-191.222	-40.207	3.515

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
2350 K, melting point of B; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2473 K: $Cp° = 50.500 + 27.500\times10^{-3}T - 20.400\times10^{5}T^{-2}$
$H°-H°_{298} = 50.500\times10^{-3}T + 13.750\times10^{-6}T^{2} + 20.400\times10^{2}T^{-1} - 23.121$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -43.106 - 10.768\times10^{-3}T + 3.719\times10^{-6}T^{2} - 600.600T^{-1}$
$\Delta Gf° = -43.106 + 10.768\times10^{-3}T\ln T - 3.719\times10^{-6}T^{2} - 300.300T^{-1} - 77.984\times10^{-3}T$
933.61-2350 K: $\Delta Hf° = -44.373 - 13.766\times10^{-3}T + 5.446\times10^{-6}T^{2} - 618.000T^{-1}$
$\Delta Gf° = -44.373 + 13.766\times10^{-3}T\ln T - 5.446\times10^{-6}T^{2} - 309.000T^{-1} - 95.508\times10^{-3}T$
2350-2473 K: $\Delta Hf° = -157.052 - 47.090\times10^{-3}T + 13.750\times10^{-6}T^{2} + 2040.000T^{-1}$
$\Delta Gf° = -157.052 + 47.090\times10^{-3}T\ln T - 13.750\times10^{-6}T^{2} + 1020.000T^{-1} - 286.952\times10^{-3}T$

Source: Data from Barin (23) who estimated all except enthalpy of formation at 298 K.

$AlBO_2(g)$
Aluminum Boron Dioxide (ideal gas)
[Formation: $Al(c,l) + B(\beta) + O_2(g) = AlBO_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	12.627	64.420	64.420	0	-129.400	-131.555	96.431
300	12.663	64.498	64.421	.023	-129.406	-131.568	95.846
400	14.289	68.377	64.937	1.376	-129.678	-132.249	72.256
500	15.445	71.697	65.965	2.866	-129.950	-132.857	58.071
600	16.294	74.592	67.169	4.454	-130.243	-133.414	48.595
700	16.936	77.154	68.415	6.117	-130.558	-133.916	41.810
800	17.432	79.449	69.653	7.837	-130.901	-134.372	36.708
900	17.821	81.526	70.859	9.600	-131.281	-134.785	32.730
933.61	17.925	82.181	71.255	10.201	-131.417	-134.913	31.582
933.61	17.925	82.181	71.255	10.201	-133.997	-134.913	31.581
1000	18.129	83.420	72.022	11.398	-134.248	-134.969	29.497
1100	18.377	85.160	73.138	13.224	-134.624	-135.029	26.827
1200	18.578	86.768	74.208	15.072	-135.002	-135.046	24.595
1300	18.743	88.261	75.232	16.938	-135.385	-135.031	22.701
1400	18.879	89.655	76.212	18.820	-135.774	-134.989	21.072
1500	18.993	90.962	77.153	20.713	-136.173	-134.917	19.657
1600	19.089	92.191	78.055	22.618	-136.582	-134.832	18.417
1700	19.171	93.351	78.921	24.531	-137.002	-134.709	17.318
1800	19.240	94.448	79.753	26.451	-137.435	-134.548	16.336
1900	19.300	95.490	80.554	28.379	-137.880	-134.373	15.456
2000	19.353	96.482	81.326	30.311	-138.340	-134.192	14.664

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 15.927 + 2.232\times10^{-3}T - 3.525\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.927\times10^{-3}T + 1.116\times10^{-6}T^{2} + 3.525\times10^{2}T^{-1} - 6.030$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -129.401 - 0.618\times10^{-3}T - 1.806\times10^{-6}T^{2} + 103.200T^{-1}$

$\Delta Gf^\circ = -129.401 + 0.618\times10^{-3}T\ln T + 1.806\times10^{-6}T^{2} + 51.600T^{-1} - 11.865\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -130.669 - 3.616\times10^{-3}T - 0.079\times10^{-6}T^{2} + 85.800T^{-1}$

$\Delta Gf^\circ = -130.669 + 3.616\times10^{-3}T\ln T + 0.079\times10^{-6}T^{2} + 42.900T^{-1} - 29.388\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

AlC(g)
Aluminum Carbide (ideal gas)
[Formation: Al(c,l) + C(c) = AlC(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	7.710	53.380	53.380	0	164.800	151.314	-110.915
300	7.718	53.428	53.381	.014	164.799	151.230	-110.169
400	8.106	55.705	53.688	.807	164.750	146.713	-80.159
500	8.366	57.544	54.282	1.631	164.633	142.215	-62.162
600	8.540	59.085	54.957	2.477	164.451	137.750	-50.175
700	8.660	60.411	55.644	3.337	164.205	133.318	-41.623
800	8.747	61.574	56.314	4.208	163.898	128.926	-35.220
900	8.813	62.608	56.957	5.086	163.529	124.574	-30.250
933.61	8.830	62.931	57.166	5.382	163.392	123.123	-28.822
933.61	8.830	62.931	57.166	5.382	160.812	123.123	-28.822
1000	8.864	63.539	57.569	5.970	160.556	120.451	-26.324
1100	8.906	64.386	58.151	6.859	160.162	116.470	-23.140
1200	8.940	65.163	58.704	7.751	159.757	112.505	-20.490
1300	8.970	65.879	59.228	8.646	159.343	108.583	-18.254
1400	8.996	66.545	59.727	9.545	158.924	104.695	-16.343
1500	9.019	67.166	60.203	10.445	158.497	100.836	-14.692
1600	9.040	67.749	60.657	11.348	158.067	97.006	-13.250
1700	9.059	68.298	61.090	12.253	157.631	93.201	-11.982
1800	9.077	68.816	61.505	13.160	157.192	89.426	-10.858
1900	9.093	69.307	61.902	14.069	156.750	85.675	-9.855
2000	9.109	69.774	62.285	14.979	156.303	81.945	-8.954
2100	9.125	70.219	62.652	15.890	155.853	78.235	-8.142
2200	9.139	70.644	63.006	16.804	155.402	74.550	-7.406
2300	9.153	71.050	63.347	17.718	154.947	70.889	-6.736
2400	9.167	71.440	63.676	18.634	154.489	67.242	-6.123
2500	9.180	71.815	63.994	19.552	154.031	63.616	-5.561

*Data estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp^\circ = 8.652 + 0.254\times10^{-3}T - 0.905\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.652\times10^{-3}T + 0.127\times10^{-6}T^{2} + 0.905\times10^{2}T^{-1} - 2.894$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = 165.065 + 0.542\times10^{-3}T - 2.366\times10^{-6}T^{2} - 64.400T^{-1}$

$\Delta Gf^\circ = 165.065 - 0.542\times10^{-3}T\ln T + 2.366\times10^{-6}T^{2} - 32.200T^{-1} - 43.375\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = 163.797 - 2.456\times10^{-3}T - 0.639\times10^{-6}T^{2} - 81.800T^{-1}$

$\Delta Gf^\circ = 163.797 + 2.456\times10^{-3}T\ln T + 0.639\times10^{-6}T^{2} - 40.900T^{-1} - 60.898\times10^{-3}T$

2000-2500 K: $\Delta Hf^\circ = 165.789 - 4.579\times10^{-3}T - 0.007\times10^{-6}T^{2} - 629.500T^{-1}$

$\Delta Gf^\circ = 165.789 + 4.579\times10^{-3}T\ln T + 0.007\times10^{-6}T^{2} - 314.750T^{-1} - 76.698\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$AlC_2(g)$
Aluminum Dicarbide (ideal gas)
[Formation: $Al(c,l) + 2C(c) = AlC_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	11.429	60.429	60.429	0	163.862	148.683	-108.987
300	11.440	60.500	60.430	.021	163.864	148.589	-108.245
400	11.974	63.866	60.884	1.193	163.950	143.482	-78.394
500	12.422	66.588	61.762	2.413	163.912	138.366	-60.479
600	12.805	68.887	62.762	3.675	163.769	133.272	-48.544
700	13.128	70.886	63.783	4.972	163.536	128.205	-40.027
800	13.397	72.657	64.783	6.299	163.226	123.179	-33.650
900	13.618	74.248	65.748	7.650	162.843	118.192	-28.701
933.61	13.679	74.748	66.063	8.109	162.700	116.528	-27.278
933.61	13.679	74.748	66.063	8.109	160.120	116.528	-27.278
1000	13.799	75.693	66.672	9.021	159.850	113.436	-24.791
1100	13.949	77.015	67.552	10.409	159.431	108.837	-21.624
1200	14.072	78.234	68.392	11.810	158.997	104.235	-18.984
1300	14.175	79.365	69.194	13.222	158.550	99.687	-16.759
1400	14.261	80.419	69.959	14.644	158.095	95.176	-14.857
1500	14.333	81.405	70.689	16.074	157.630	90.699	-13.215
1600	14.394	82.332	71.388	17.511	157.160	86.254	-11.782
1700	14.446	83.206	72.057	18.953	156.679	81.835	-10.520
1800	14.491	84.033	72.700	20.400	156.193	77.448	-9.403
1900	14.530	84.818	73.317	21.851	155.701	73.087	-8.407
2000	14.564	85.564	73.912	23.305	155.200	68.752	-7.513

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 12.240 + 1.478\times10^{-3}T - 1.113\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.240\times10^{-3}T + 0.739\times10^{-6}T^{2} + 1.113\times10^{2}T^{-1} - 4.088$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = 164.628 + 0.612\times10^{-3}T - 2.520\times10^{-6}T^{2} - 215.900T^{-1}$

$\Delta Gf^\circ = 164.628 - 0.612\times10^{-3}T\ln T + 2.520\times10^{-6}T^{2} - 107.950T^{-1} - 49.527\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = 163.360 - 2.386\times10^{-3}T - 0.793\times10^{-6}T^{2} - 233.300T^{-1}$

$\Delta Gf^\circ = 163.360 + 2.386\times10^{-3}T\ln T + 0.793\times10^{-6}T^{2} - 116.650T^{-1} - 67.050\times10^{-3}T$

Source: Data from Gurvich (196) who estimated all except enthalpy of formation at 298 K.

$Al_2C_2(g)$
Dialuminum Dicarbide (ideal gas)
[Formation: $2Al(c,l) + 2C(c) = Al_2C_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.172	67.994	67.994	0	135.023	119.609	-87.675
300	16.191	68.094	67.994	.030	135.023	119.513	-87.064
400	17.045	72.875	68.640	1.694	135.003	114.343	-62.474
500	17.695	76.752	69.888	3.432	134.859	109.192	-47.727
600	18.216	80.026	71.311	5.229	134.600	104.085	-37.913
700	18.638	82.866	72.763	7.072	134.231	99.027	-30.917
800	18.982	85.379	74.187	8.954	133.757	94.028	-25.687
900	19.262	87.631	75.558	10.866	133.175	89.092	-21.634
933.61	19.339	88.339	76.005	11.515	132.957	87.450	-20.471
933.61	19.339	88.339	76.005	11.515	127.797	87.450	-20.471
1000	19.490	89.673	76.869	12.804	127.399	84.594	-18.488
1100	19.677	91.539	78.118	14.763	126.792	80.364	-15.967
1200	19.831	93.258	79.309	16.739	126.174	76.151	-13.869
1300	19.959	94.851	80.445	18.728	125.545	72.004	-12.105
1400	20.065	96.334	81.527	20.730	124.911	67.911	-10.601
1500	20.155	97.722	82.561	22.741	124.268	63.860	-9.304
1600	20.231	99.025	83.550	24.760	123.621	59.856	-8.176
1700	20.296	100.253	84.496	26.787	122.966	55.889	-7.185
1800	20.352	101.415	85.404	28.819	122.306	51.964	-6.309
1900	20.400	102.517	86.276	30.857	121.642	48.076	-5.530
2000	20.442	103.564	87.115	32.899	120.970	44.222	-4.832

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:

$$Cp° = 17.440 + 1.998\times10^{-3}T - 1.656\times10^{5}T^{-2}$$
$$H°- H°_{298} = 17.440\times10^{-3}T + 0.999\times10^{-6}T^{2} + 1.656\times10^{2}T^{-1} - 5.844$$

Formation equations (kcal/mol):

298.15-933.61 K:

$$\Delta Hf° = 135.497 + 1.220\times10^{-3}T - 3.987\times10^{-6}T^{2} - 144.200T^{-1}$$
$$\Delta Gf° = 135.497 - 1.220\times10^{-3}T\ln T + 3.987\times10^{-6}T^{2} - 72.100T^{-1} - 46.715\times10^{-3}T$$

933.61-2000 K:

$$\Delta Hf° = 132.962 - 4.776\times10^{-3}T - 0.533\times10^{-6}T^{2} - 179.000T^{-1}$$
$$\Delta Gf° = 132.962 + 4.776\times10^{-3}T\ln T + 0.533\times10^{-6}T^{2} - 89.500T^{-1} - 81.762\times10^{-3}T$$

Source: Data from Gurvich (196) who estimated all except enthalpy of formation at 298 K.

$Al_4C_3(c)$
Tetraaluminum Tricarbide
[Formation: $4Al(c,l) + 3C(c) = Al_4C_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	27.909	21.264	21.264	0	-49.900	-46.932	34.401
300	28.054	21.437	21.264	.052	-49.904	-46.914	34.177
400	33.404	30.343	22.443	3.160	-49.920	-45.910	25.084
500	36.207	38.124	24.820	6.652	-49.875	-44.913	19.631
600	38.048	44.898	27.615	10.370	-49.892	-43.914	15.995
700	39.453	50.872	30.518	14.248	-50.014	-42.909	13.397
800	40.639	56.219	33.402	18.254	-50.261	-41.879	11.441
900	41.705	61.068	36.210	22.372	-50.644	-40.815	9.911
933.61	42.039	62.603	37.133	23.779	-50.802	-40.444	9.467
933.61	42.039	62.603	37.133	23.779	-61.122	-40.444	9.467
1000	42.700	65.514	38.922	26.592	-61.345	-38.968	8.516
1100	43.650	69.629	41.529	30.910	-61.635	-36.686	7.289
1200	44.567	73.466	44.032	35.321	-61.874	-34.436	6.272
1300	45.456	77.069	46.436	39.823	-62.058	-32.145	5.404
1400	46.319	80.469	48.747	44.411	-62.183	-29.837	4.658
1500	47.154	83.694	50.971	49.085	-62.249	-27.528	4.011
1600	47.959	86.763	53.112	53.841	-62.251	-25.209	3.443
1700	48.729	89.694	55.179	58.676	-62.198	-22.901	2.944
1800	49.459	92.500	57.174	63.586	-62.085	-20.588	2.500
1900	50.145	95.193	59.106	68.566	-61.917	-18.283	2.103
2000	50.781	97.781	60.974	73.613	-61.700	-15.992	1.748

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 36.103 + 7.590\times10^{-3}T - 9.296\times10^{5}T^{-2}$

$H°-H°_{298} = 36.103\times10^{-3}T + 3.795\times10^{-6}T^{2} + 9.296\times10^{2}T^{-1} - 14.219$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -53.178 + 7.181\times10^{-3}T - 5.411\times10^{-6}T^{2} + 482.300T^{-1}$

$\Delta Gf° = -53.178 - 7.181\times10^{-3}T\ln T + 5.411\times10^{-6}T^{2} + 241.150T^{-1} + 57.538\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = -58.248 - 4.811\times10^{-3}T + 1.497\times10^{-6}T^{2} + 412.700T^{-1}$

$\Delta Gf° = -58.248 + 4.811\times10^{-3}T\ln T - 1.497\times10^{-6}T^{2} + 206.350T^{-1} - 12.556\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from Furukawa (164). High-temperature data based on Furukawa (164) and Binford (44).

AlH(g)
Aluminum Hydride (ideal gas)
[Formation: $Al(c,l) + 0.5H_2(g) = AlH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.020	44.875	44.875	0	61.960	55.253	-40.501
300	7.022	44.918	44.875	.013	61.955	55.211	-40.221
400	7.180	46.958	45.153	.722	61.719	52.998	-28.956
500	7.408	48.584	45.682	1.451	61.475	50.845	-22.224
600	7.650	49.956	46.283	2.204	61.227	48.744	-17.755
700	7.874	51.152	46.893	2.981	60.971	46.685	-14.575
800	8.068	52.217	47.494	3.778	60.696	44.661	-12.201
900	8.232	53.177	48.074	4.593	60.396	42.674	-10.362
933.61	8.278	53.480	48.263	4.870	60.288	42.014	-9.835
933.61	8.278	53.480	48.263	4.870	57.708	42.014	-9.835
1000	8.370	54.051	48.627	5.424	57.518	40.906	-8.940
1100	8.486	54.855	49.158	6.267	57.238	39.257	-7.800
1200	8.585	55.598	49.665	7.120	56.965	37.634	-6.854
1300	8.669	56.288	50.147	7.983	56.695	36.035	-6.058
1400	8.742	56.933	50.609	8.854	56.430	34.457	-5.379
1500	8.806	57.539	51.052	9.731	56.164	32.894	-4.793
1600	8.863	58.109	51.475	10.615	55.900	31.352	-4.282
1700	8.913	58.648	51.881	11.504	55.637	29.826	-3.834
1800	8.959	59.158	52.271	12.397	55.373	28.316	-3.438
1900	9.001	59.644	52.647	13.295	55.108	26.820	-3.085
2000	9.039	60.107	53.008	14.197	54.844	25.337	-2.769

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.065 + 1.162\times10^{-3}T - 0.348\times10^{5}T^{-2}$

$H°-H°_{298} = 7.065\times10^{-3}T + 0.581\times10^{-6}T^{2} + 0.348\times10^{2}T^{-1} - 2.275$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = 62.103 - 0.755\times10^{-3}T - 1.355\times10^{-6}T^{2} + 60.450T^{-1}$

$\Delta Gf° = 62.103 + 0.755\times10^{-3}T\ln T + 1.355\times10^{-6}T^{2} + 30.225T^{-1} - 28.020\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = 60.835 - 3.753\times10^{-3}T + 0.371\times10^{-6}T^{2} + 43.050T^{-1}$

$\Delta Gf° = 60.835 + 3.753\times10^{-3}T\ln T - 0.371\times10^{-6}T^{2} + 21.525T^{-1} - 45.544\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data from JANAF (127).

$AlH_2(g)$
Aluminum Dihydride (ideal gas)
[Formation: $Al(c,l) + H_2(g) = AlH_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.789	50.957	50.957	0	59.048	55.180	-40.447
300	8.559	51.010	50.957	.016	59.040	55.156	-40.180
400	9.088	53.543	51.298	.898	58.630	53.924	-29.462
500	9.646	55.631	51.963	1.834	58.243	52.792	-23.075
600	10.197	57.439	52.727	2.827	57.885	51.737	-18.845
700	10.704	59.050	53.519	3.872	57.546	50.739	-15.841
800	11.149	60.508	54.302	4.965	57.214	49.789	-13.602
900	11.529	61.844	55.066	6.100	56.878	48.881	-11.870
933.61	11.637	62.269	55.318	6.489	56.762	48.584	-11.373
933.61	11.637	62.269	55.318	6.489	54.182	48.584	-11.373
1000	11.849	63.076	55.807	7.269	53.979	48.192	-10.532
1100	12.118	64.218	56.520	8.468	53.693	47.628	-9.463
1200	12.343	65.283	57.207	9.691	53.421	47.089	-8.576
1300	12.534	66.278	57.866	10.936	53.161	46.573	-7.829
1400	12.696	67.213	58.501	12.197	52.907	46.075	-7.193
1500	12.835	68.094	59.111	13.474	52.658	45.595	-6.643
1600	12.957	68.926	59.699	14.764	52.412	45.132	-6.165
1700	13.065	69.715	60.265	16.065	52.167	44.685	-5.745
1800	13.163	70.465	60.812	17.376	51.922	44.250	-5.373
1900	13.252	71.179	61.338	18.697	51.678	43.833	-5.042
2000	13.334	71.861	61.848	20.026	51.433	43.425	-4.745

*Enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.830 + 2.746\times10^{-3}T - 0.765\times10^{5}T^{-2}$

$H°-H°_{298} = 8.830\times10^{-3}T + 1.373\times10^{-6}T^{2} + 0.765\times10^{2}T^{-1} - 3.011$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = 59.408 - 2.218\times10^{-3}T - 0.773\times10^{-6}T^{2} + 110.400T^{-1}$

$\Delta Gf° = 59.408 + 2.218\times10^{-3}T\ln T + 0.773\times10^{-6}T^{2} + 55.200T^{-1} - 27.669\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = 58.140 - 5.216\times10^{-3}T + 0.954\times10^{-6}T^{2} + 93.000T^{-1}$

$\Delta Gf° = 58.140 + 5.216\times10^{-3}T\ln T - 0.954\times10^{-6}T^{2} + 46.500T^{-1} - 45.193\times10^{-3}T$

Source: Data from Gurvich (196) who estimated enthalpy of formation at 298 K.

AlH_3(hexagonal)
Aluminum Trihydride
[Formation: $Al(c) + 1.5H_2(g) = AlH_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	9.610	7.180	7.180	0	-2.725	11.111	-8.145
300*	9.669	7.239	7.180	.018	-2.737	11.197	-8.157
400	11.950	10.368	7.591	1.111	-3.284	15.930	-8.703
500	13.324	13.192	8.434	2.379	-3.688	20.781	-9.083

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp° = 11.803 + 5.832\times10^{-3}T - 3.495\times10^{5}T^{-2}$

$H°-H°_{298} = 11.803\times10^{-3}T + 2.916\times10^{-6}T^{2} + 3.495\times10^{2}T^{-1} - 4.951$

Formation equations (kcal/mol):

298.15-500 K: $\Delta Hf° = -3.351 - 2.473\times10^{-3}T + 0.560\times10^{-6}T^{2} + 391.650T^{-1}$

$\Delta Gf° = -3.351 + 2.473\times10^{-3}T\ln T - 0.560\times10^{-6}T^{2} + 195.825T^{-1} + 32.380\times10^{-3}T$

Source: Data from Gurvich (196) who estimated all above 298 K.

$AlH_3(g)$
Aluminum Trihydride (ideal gas)
[Formation: $Al(c,l) + 1.5H_2(g) = AlH_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	9.574	49.346	49.346	0	49.747	51.011	-37.392
300	9.598	49.406	49.346	.018	49.735	51.019	-37.167
400	10.895	52.345	49.738	1.043	49.121	51.543	-28.161
500	12.133	54.911	50.521	2.195	48.600	52.210	-22.821
600	13.253	57.224	51.449	3.465	48.169	52.974	-19.296
700	14.227	59.342	52.428	4.840	47.809	53.805	-16.798
800	15.053	61.297	53.415	6.306	47.497	54.684	-14.939
900	15.742	63.111	54.392	7.847	47.212	55.599	-13.501
933.61	15.934	63.692	54.717	8.379	47.118	55.914	-13.089
933.61	15.934	63.692	54.717	8.379	44.538	55.914	-13.089
1000	16.314	64.800	55.350	9.450	44.388	56.727	-12.397
1100	16.787	66.378	56.282	11.106	44.195	57.970	-11.517
1200	17.180	67.856	57.185	12.805	44.032	59.231	-10.787
1300	17.507	69.245	58.060	14.540	43.889	60.503	-10.171
1400	17.783	70.552	58.906	16.305	43.761	61.787	-9.645
1500	18.015	71.787	59.724	18.095	43.641	63.077	-9.190
1600	18.212	72.956	60.515	19.906	43.528	64.375	-8.793
1700	18.381	74.066	61.280	21.736	43.418	65.683	-8.444
1800	18.526	75.120	62.019	23.582	43.310	66.997	-8.134
1900	18.652	76.126	62.736	25.441	43.201	68.316	-7.858
2000	18.761	77.085	63.430	27.311	43.089	69.640	-7.610

*Enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.523 + 4.504\times10^{-3}T - 2.926\times10^{5}T^{-2}$

$H°-H°_{298} = 11.523\times10^{-3}T + 2.252\times10^{-6}T^{2} + 2.926\times10^{2}T^{-1} - 4.617$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = 49.454 - 2.753\times10^{-3}T - 0.104\times10^{-6}T^{2} + 334.750T^{-1}$

$\Delta Gf° = 49.454 + 2.753\times10^{-3}T\ln T + 0.104\times10^{-6}T^{2} + 167.375T^{-1} - 12.377\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = 48.187 - 5.751\times10^{-3}T + 1.623\times10^{-6}T^{2} + 317.350T^{-1}$

$\Delta Gf° = 48.187 + 5.751\times10^{-3}T\ln T - 1.623\times10^{-6}T^{2} + 158.675T^{-1} - 29.900\times10^{-3}T$

Source: Data from Gurvich (196) who estimated enthalpy of formation at 298 K.

$AlN(c)$
Aluminum Nitride
[Formation: $Al(c,l) + 0.5N_2(g) = AlN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.203	4.800	4.800	0	-75.600	-68.188	49.982
300	7.238	4.845	4.802	.013	-75.604	-68.142	49.641
400	8.709	7.138	5.103	.814	-75.750	-65.630	35.858
500	9.726	9.197	5.719	1.739	-75.800	-63.091	27.577
600	10.437	11.037	6.455	2.749	-75.798	-60.549	22.055
700	10.935	12.686	7.230	3.819	-75.773	-58.009	18.111
800	11.278	14.170	8.006	4.931	-75.752	-55.473	15.154
900	11.506	15.512	8.766	6.071	-75.752	-52.938	12.855
933.61	11.556	15.935	9.017	6.459	-75.758	-52.086	12.193
933.61	11.556	15.935	9.017	6.459	-78.338	-52.086	12.193
1000	11.655	16.733	9.503	7.230	-78.330	-50.220	10.975
1100	11.749	17.848	10.212	8.400	-78.313	-47.410	9.419
1200	11.811	18.873	10.891	9.578	-78.294	-44.601	8.123
1300	11.857	19.821	11.543	10.762	-78.274	-41.795	7.026
1400	11.898	20.701	12.166	11.949	-78.257	-38.989	6.086
1500	11.943	21.523	12.762	13.141	-78.239	-36.185	5.272
1600	11.994	22.296	13.335	14.338	-78.218	-33.383	4.560
1700	12.051	23.024	13.882	15.541	-78.196	-30.580	3.931
1800	12.109	23.715	14.410	16.749	-78.171	-27.780	3.373
1900	12.157	24.371	14.917	17.962	-78.144	-24.981	2.873
2000	12.184	24.995	15.406	19.179	-78.115	-22.183	2.424

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.011 + 0.760\times10^{-3}T - 3.586\times10^{5}T^{-2}$

$H°- H°_{298} = 11.011\times10^{-3}T + 0.380\times10^{-6}T^{2} + 3.586\times10^{2}T^{-1} - 4.519$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -77.671 + 3.161\times10^{-3}T - 1.641\times10^{-6}T^{2} + 379.950T^{-1}$

$\Delta Gf° = -77.671 - 3.161\times10^{-3}T\ln T + 1.641\times10^{-6}T^{2} + 189.975T^{-1} + 47.187\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = -78.938 + 0.162\times10^{-3}T + 0.086\times10^{-6}T^{2} + 362.550T^{-1}$

$\Delta Gf° = -78.938 - 0.162\times10^{-3}T\ln T - 0.086\times10^{-6}T^{2} + 181.275T^{-1} + 29.664\times10^{-3}T$

Source: Data based on Mah (319).

AlN(g)
Aluminum Nitride (ideal gas)
[Formation: $Al(c,l) + 0.5N_2(g) = AlN(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.736	54.599	54.599	0	125.000	117.565	-86.176
300	7.745	54.647	54.600	.014	124.996	117.518	-85.611
400	8.131	56.932	54.910	.809	124.845	115.048	-62.858
500	8.387	58.775	55.503	1.636	124.697	112.617	-49.224
600	8.558	60.321	56.181	2.484	124.537	110.216	-40.146
700	8.677	61.649	56.869	3.346	124.353	107.844	-33.670
800	8.763	62.814	57.542	4.218	124.135	105.499	-28.821
900	8.827	63.850	58.186	5.098	123.876	103.185	-25.056
933.61	8.844	64.174	58.395	5.395	123.778	102.414	-23.974
933.61	8.844	64.174	58.395	5.395	121.198	102.414	-23.974
1000	8.878	64.783	58.800	5.983	121.023	101.083	-22.091
1100	8.920	65.631	59.383	6.873	120.760	99.102	-19.689
1200	8.954	66.409	59.936	7.767	120.495	97.145	-17.692
1300	8.984	67.127	60.462	8.664	120.228	95.210	-16.006
1400	9.010	67.793	60.962	9.564	119.958	93.297	-14.564
1500	9.034	68.416	61.439	10.466	119.687	91.400	-13.317
1600	9.055	69.000	61.894	11.370	119.413	89.522	-12.228
1700	9.075	69.549	62.327	12.277	119.140	87.664	-11.270
1800	9.093	70.068	62.743	13.185	118.865	85.821	-10.420
1900	9.111	70.560	63.142	14.095	118.590	83.993	-9.661
2000	9.127	71.028	63.525	15.007	118.314	82.179	-8.980

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.616 + 0.306 \times 10^{-3}T - 0.863 \times 10^{5}T^{-2}$

$H°-H°_{298} = 8.616 \times 10^{-3}T + 0.153 \times 10^{-6}T^{2} + 0.863 \times 10^{2}T^{-1} - 2.872$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = 124.577 + 0.766 \times 10^{-3}T - 1.868 \times 10^{-6}T^{2} + 107.650T^{-1}$

$\Delta Gf° = 124.577 - 0.766 \times 10^{-3}T\ln T + 1.868 \times 10^{-6}T^{2} + 53.825T^{-1} - 20.320 \times 10^{-3}T$

933.61-2000 K: $\Delta Hf° = 123.309 - 2.232 \times 10^{-3}T - 0.142 \times 10^{-6}T^{2} + 90.250T^{-1}$

$\Delta Gf° = 123.309 + 2.232 \times 10^{-3}T\ln T + 0.142 \times 10^{-6}T^{2} + 45.125T^{-1} - 37.843 \times 10^{-3}T$

Source: Data from JANAF (131).

AlOCl(c)
Aluminum Oxychloride
[Formation: $Al(c) + 0.5O_2(g) + 0.5Cl_2(g) = AlOCl(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.600	13.000	13.000	0	-189.200	-175.806	128.868
300	13.650	13.084	13.001	.025	-189.200	-175.723	128.013
400	15.370	17.293	13.563	1.492	-189.101	-171.243	93.562
500	16.540	20.858	14.674	3.092	-188.917	-166.798	72.906
600	17.360	23.952	15.969	4.790	-188.682	-162.394	59.151

*Data except enthalpy of formation at 298 K estimated. Decomposes near 500 K.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 16.279 + 3.182\times10^{-3}T - 3.225\times10^{5}T^{-2}$

$H°- H°_{298} = 16.279\times10^{-3}T + 1.591\times10^{-6}T^{2} + 3.225\times10^{2}T^{-1} - 6.077$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = -191.202 + 3.658\times10^{-3}T - 0.431\times10^{-6}T^{2} + 283.150T^{-1}$

$\Delta Gf° = -191.202 - 3.658\times10^{-3}T\ln T + 0.431\times10^{-6}T^{2} + 141.575T^{-1} + 70.762\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data are those estimated by JANAF (127).

AlOCl(g)
Aluminum Oxychloride (ideal gas)
[Formation: $Al(c,l) + 0.5O_2(g) + 0.5Cl_2(g) = AlOCl(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	11.967	59.471	59.471	0	-83.200	-83.661	61.325
300	11.989	59.545	59.472	.022	-83.203	-83.665	60.949
400	12.935	63.135	59.955	1.272	-83.321	-83.800	45.786
500	13.511	66.089	60.895	2.597	-83.412	-83.908	36.676
600	13.877	68.587	61.974	3.968	-83.504	-83.997	30.596
700	14.120	70.745	63.076	5.368	-83.614	-84.071	26.248
800	14.288	72.642	64.156	6.789	-83.754	-84.128	22.983
900	14.409	74.333	65.195	8.224	-83.931	-84.166	20.438
933.61	14.439	74.862	65.534	8.709	-84.000	-84.173	19.704
933.61	14.439	74.862	65.534	8.709	-86.580	-84.173	19.704
1000	14.498	75.855	66.185	9.670	-86.695	-83.997	18.357
1100	14.565	77.241	67.129	11.123	-86.869	-83.721	16.634
1200	14.617	78.510	68.025	12.582	-87.043	-83.425	15.194
1300	14.658	79.682	68.877	14.046	-87.217	-83.118	13.973
1400	14.691	80.769	69.688	15.514	-87.393	-82.794	12.925
1500	14.718	81.784	70.461	16.984	-87.569	-82.462	12.015
1600	14.740	82.734	71.198	18.457	-87.748	-82.114	11.216
1700	14.758	83.629	71.904	19.932	-87.927	-81.757	10.510
1800	14.774	84.473	72.579	21.409	-88.109	-81.389	9.882
1900	14.787	85.272	73.226	22.887	-88.293	-81.008	9.318
2000	14.798	86.031	73.848	24.366	-88.480	-80.622	8.810

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.257 + 0.364\times10^{-3}T - 2.132\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.257\times10^{-3}T + 0.182\times10^{-6}T^{2} + 2.132\times10^{2}T^{-1} - 4.982$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -84.107 + 1.636\times10^{-3}T - 1.840\times10^{-6}T^{2} + 173.850T^{-1}$

$\Delta Gf^\circ = -84.107 - 1.636\times10^{-3}T\ln T + 1.840\times10^{-6}T^{2} + 86.925T^{-1} + 9.294\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -85.375 - 1.362\times10^{-3}T - 0.113\times10^{-6}T^{2} + 156.450T^{-1}$

$\Delta Gf^\circ = -85.375 + 1.362\times10^{-3}T\ln T + 0.113\times10^{-6}T^{2} + 78.225T^{-1} - 8.230\times10^{-3}T$

Source: Data from JANAF (127).

AlOF(g)
Aluminum Oxyfluoride (ideal gas)
[Formation: $Al(c,l) + 0.5O_2(g) + 0.5F_2(g) = AlOF(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	11.187	56.693	56.693	0	-139.000	-139.356	102.149
300	11.212	56.762	56.693	.021	-139.004	-139.358	101.521
400	12.307	60.149	57.146	1.201	-139.161	-139.451	76.191
500	13.021	62.977	58.039	2.469	-139.285	-139.508	60.978
600	13.495	65.396	59.068	3.797	-139.400	-139.541	50.827
700	13.817	67.502	60.126	5.163	-139.529	-139.555	43.570
800	14.045	69.363	61.167	6.557	-139.684	-139.550	38.123
900	14.209	71.027	62.171	7.970	-139.874	-139.522	33.880
933.61	14.250	71.549	62.500	8.448	-139.946	-139.507	32.657
933.61	14.250	71.549	62.500	8.448	-142.526	-139.507	32.657
1000	14.332	72.531	63.133	9.398	-142.649	-139.288	30.441
1100	14.425	73.901	64.050	10.836	-142.833	-138.943	27.605
1200	14.498	75.160	64.925	12.282	-143.015	-138.582	25.239
1300	14.555	76.322	65.757	13.735	-143.197	-138.204	23.234
1400	14.601	77.403	66.551	15.193	-143.380	-137.814	21.513
1500	14.639	78.411	67.308	16.655	-143.563	-137.410	20.020
1600	14.670	79.357	68.032	18.120	-143.749	-136.994	18.712
1700	14.696	80.247	68.725	19.588	-143.935	-136.566	17.557
1800	14.718	81.088	69.389	21.059	-144.122	-136.127	16.528
1900	14.737	81.884	70.025	22.532	-144.312	-135.676	15.606
2000	14.753	82.641	70.638	24.006	-144.505	-135.219	14.776

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.862 + 0.582x10^{-3}T - 2.532x10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.862x10^{-3}T + 0.291x10^{-6}T^{2} + 2.532x10^{2}T^{-1} - 5.008$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -139.923 + 1.401x10^{-3}T - 1.775x10^{-6}T^{2} + 197.750T^{-1}$

$\Delta Gf^\circ = -139.923 - 1.401x10^{-3}TlnT + 1.775x10^{-6}T^{2} + 98.875T^{-1} + 8.244x10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -141.191 - 1.597x10^{-3}T - 0.048x10^{-6}T^{2} + 180.350T^{-1}$

$\Delta Gf^\circ = -141.191 + 1.597x10^{-3}TlnT + 0.048x10^{-6}T^{2} + 90.175T^{-1} - 9.279x10^{-3}T$

Source: Data from Chase (82) who estimated all except enthalpy of formation at 298 K.

$AlOF_2(g)$
Aluminum Difluoride Oxide (ideal gas)
[Formation: $Al(c,l) + 0.5O_2(g) + F_2(g) = AlOF_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.150	69.931	69.931	0	-265.000	-262.081	192.108
300	15.182	70.025	69.932	.028	-265.003	-262.063	190.911
400	16.576	74.597	70.545	1.621	-265.133	-261.061	142.635
500	17.493	78.402	71.748	3.327	-265.220	-260.033	113.659
600	18.098	81.648	73.133	5.109	-265.296	-258.987	94.335
700	18.509	84.471	74.555	6.941	-265.383	-257.928	80.528
800	18.796	86.962	75.953	8.807	-265.497	-256.857	70.169
900	19.004	89.189	77.303	10.697	-265.646	-255.769	62.108
933.61	19.056	89.887	77.744	11.337	-265.704	-255.400	59.786
933.61	19.056	89.887	77.744	11.337	-268.284	-255.400	59.786
1000	19.158	91.199	78.593	12.606	-268.380	-254.480	55.616
1100	19.276	93.031	79.824	14.528	-268.522	-253.083	50.282
1200	19.368	94.712	80.995	16.460	-268.665	-251.673	45.835
1300	19.441	96.266	82.111	18.401	-268.806	-250.251	42.071
1400	19.503	97.709	83.175	20.348	-268.950	-248.820	38.842
1500	19.555	99.056	84.189	22.301	-269.094	-247.377	36.042
1600	19.601	100.320	85.158	24.259	-269.239	-245.925	33.591
1700	19.644	101.509	86.085	26.221	-269.385	-244.461	31.427
1800	19.684	102.633	86.974	28.187	-269.534	-242.991	29.503
1900	19.723	103.698	87.825	30.158	-269.682	-241.510	27.780
2000	19.761	104.711	88.645	32.132	-269.833	-240.025	26.228

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.550 + 0.758\times10^{-3}T - 3.224\times10^{5}T^{-2}$
$H°- H°_{298} = 18.550\times10^{-3}T + 0.379\times10^{-6}T^{2} + 3.224\times10^{2}T^{-1} - 6.646$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -266.116 + 1.835\times10^{-3}T - 1.773\times10^{-6}T^{2} + 216.700T^{-1}$
$\Delta Gf° = -266.116 - 1.835\times10^{-3}T\ln T + 1.773\times10^{-6}T^{2} + 108.350T^{-1} + 22.242\times10^{-3}T$
933.61-2000 K: $\Delta Hf° = -267.384 - 1.163\times10^{-3}T - 0.046\times10^{-6}T^{2} + 199.300T^{-1}$
$\Delta Gf° = -267.384 + 1.163\times10^{-3}T\ln T + 0.046\times10^{-6}T^{2} + 99.650T^{-1} + 4.719\times10^{-3}T$

Source: Data from Chase (82) who estimated all except enthalpy of formation at 298 K.

AlOH(g)
Aluminum Monoxyhydride (ideal gas)
[Formation: $Al(c,l) + 0.5O_2(g) + 0.5H_2(g) = AlOH(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	7.628	51.701	51.701	0	-43.000	-44.437	32.573
300	7.643	51.748	51.701	.014	-43.010	-44.446	32.378
400	8.526	54.065	52.010	.822	-43.502	-44.849	24.504
500	9.386	56.062	52.626	1.718	-43.945	-45.133	19.727
600	10.110	57.840	53.350	2.694	-44.347	-45.332	16.512
700	10.699	59.444	54.107	3.736	-44.728	-45.465	14.195
800	11.181	60.905	54.868	4.830	-45.105	-45.546	12.442
900	11.585	62.246	55.614	5.969	-45.488	-45.578	11.068
933.61	11.701	62.673	55.860	6.360	-45.620	-45.579	10.670
933.61	11.701	62.673	55.860	6.360	-48.200	-45.579	10.670
1000	11.929	63.485	56.340	7.145	-48.435	-45.385	9.919
1100	12.227	64.636	57.041	8.354	-48.767	-45.063	8.953
1200	12.487	65.712	57.720	9.590	-49.082	-44.712	8.143
1300	12.715	66.720	58.374	10.850	-49.382	-44.336	7.453
1400	12.916	67.670	59.004	12.132	-49.669	-43.937	6.859
1500	13.093	68.567	59.612	13.432	-49.947	-43.519	6.341
1600	13.251	69.418	60.199	14.750	-50.215	-43.082	5.885
1700	13.390	70.225	60.765	16.082	-50.476	-42.627	5.480
1800	13.515	70.994	61.312	17.427	-50.733	-42.158	5.119
1900	13.625	71.728	61.842	18.784	-50.985	-41.674	4.794
2000	13.725	72.429	62.353	20.152	-51.233	-41.177	4.500

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.823 + 2.980\times10^{-3}T - 1.852\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.823\times10^{-3}T + 1.490\times10^{-6}T^2 + 1.852\times10^{2}T^{-1} - 3.384$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -42.791 - 2.612\times10^{-3}T - 0.698\times10^{-6}T^2 + 188.250T^{-1}$

$\Delta Gf^\circ = -42.791 + 2.612\times10^{-3}T\ln T + 0.698\times10^{-6}T^2 + 94.125T^{-1} - 21.670\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -44.058 - 5.610\times10^{-3}T + 1.029\times10^{-6}T^2 + 170.850T^{-1}$

$\Delta Gf^\circ = -44.058 + 5.610\times10^{-3}T\ln T - 1.029\times10^{-6}T^2 + 85.425T^{-1} - 39.194\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

AlO(OH)(diaspore)
Diaspore
[Formation: $Al(c) + O_2(g) + 0.5H_2(g) = AlO(OH)(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.691	8.446	8.446	0	-238.875	-220.110	161.343
300	12.757	8.525	8.448	.023	-238.883	-219.994	160.264
400	15.673	12.621	8.986	1.454	-239.107	-213.658	116.736
500	17.724	16.351	10.091	3.130	-239.135	-207.287	90.604
600*	19.265	19.725	11.420	4.983	-239.038	-200.924	73.186
700	20.474	22.789	12.829	6.972	-238.860	-194.585	60.751

*Metastable above 572 K.

Phase change: 480.9 K, calculated decomposition temperature to α-Al_2O_3 and $H_2O(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = 13.412 + 11.408\times10^{-3}T - 3.664\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.412\times10^{-3}T + 5.704\times10^{-6}T^{2} + 3.664\times10^{2}T^{-1} - 5.735$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -239.840 - 1.638\times10^{-3}T + 3.265\times10^{-6}T^{2} + 346.850T^{-1}$

$\Delta Gf^\circ = -239.840 + 1.638\times10^{-3}T\ln T - 3.265\times10^{-6}T^{2} + 173.425T^{-1} + 55.865\times10^{-3}T$

Source: Data from Haas (198).

AlO(OH)(boehmite)
Boehmite
[Formation: $Al(c) + O_2(g) + 0.5H_2(g) = AlO(OH)(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.652	11.576	11.576	0	-236.717	-218.885	160.445
300	15.738	11.673	11.576	.029	-236.718	-218.775	159.375
400	19.628	16.764	12.244	1.808	-236.594	-212.803	116.268
500	22.481	21.466	13.626	3.920	-236.187	-206.897	90.433
600*	24.669	25.766	15.296	6.282	-235.581	-201.092	73.247
700	26.409	29.704	17.077	8.839	-234.835	-195.400	61.006

*Metastable below 572 K.

Phase change: 449.32 K, calculated decomposition temperature to α-Al_2O_3 and $H_2O(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = 15.581 + 17.160 \times 10^{-3}T - 4.484 \times 10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.581 \times 10^{-3}T + 8.580 \times 10^{-6}T^{2} + 4.484 \times 10^{2}T^{-1} - 6.912$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -238.860 + 0.531 \times 10^{-3}T + 6.141 \times 10^{-6}T^{2} + 428.850T^{-1}$

$\Delta Gf^\circ = -238.860 - 0.531 \times 10^{-3}T\ln T - 6.141 \times 10^{-6}T^{2} + 214.425T^{-1} + 69.439 \times 10^{-3}T$

Source: Data from Haas (198).

$AlO_2H(g)$
Aluminum Hydroxide Oxide (ideal gas)
[Formation: $Al(c,l) + O_2(g) + 0.5H_2(g) = AlO_2H(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.983	60.770	60.770	0	-110.000	-106.835	78.311
300	12.014	60.844	60.771	.022	-110.008	-106.816	77.814
400	13.483	64.512	61.260	1.301	-110.384	-105.692	57.747
500	14.566	67.643	62.231	2.706	-110.684	-104.482	45.669
600	15.360	70.373	63.366	4.204	-110.942	-103.217	37.596
700	15.961	72.788	64.544	5.771	-111.186	-101.910	31.817
800	16.436	74.951	65.711	7.392	-111.435	-100.569	27.474
900	16.825	76.910	66.848	9.056	-111.701	-99.195	24.088
933.61	16.936	77.529	67.221	9.623	-111.795	-98.726	23.111
933.61	16.936	77.529	67.221	9.623	-114.375	-98.726	23.111
1000	17.154	78.700	67.945	10.755	-114.538	-97.609	21.332
1100	17.436	80.349	68.999	12.485	-114.769	-95.905	19.054
1200	17.681	81.877	70.009	14.241	-114.988	-94.179	17.152
1300	17.894	83.300	70.977	16.020	-115.197	-92.436	15.540
1400	18.081	84.634	71.906	17.819	-115.398	-90.679	14.155
1500	18.246	85.887	72.796	19.636	-115.594	-88.907	12.954
1600	18.391	87.069	73.652	21.468	-115.786	-87.121	11.900
1700	18.519	88.188	74.474	23.313	-115.976	-85.323	10.969
1800	18.632	89.250	75.266	25.171	-116.164	-83.514	10.140
1900	18.733	90.260	76.029	27.039	-116.352	-81.695	9.397
2000	18.823	91.223	76.765	28.917	-116.539	-79.866	8.727

*Enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.664 + 2.542 \times 10^{-3}T - 3.056 \times 10^{5}T^{-2}$

$H°- H°_{298} = 14.664 \times 10^{-3}T + 1.271 \times 10^{-6}T^{2} + 3.056 \times 10^{2}T^{-1} - 5.510$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -110.740 - 0.386 \times 10^{-3}T - 1.169 \times 10^{-6}T^{2} + 286.050T^{-1}$

$\Delta Gf° = -110.740 + 0.386 \times 10^{-3}T\ln T + 1.169 \times 10^{-6}T^{2} + 143.025T^{-1} + 8.941 \times 10^{-3}T$

933.61-2000 K: $\Delta Hf° = -112.008 - 3.384 \times 10^{-3}T + 0.558 \times 10^{-6}T^{2} + 268.650T^{-1}$

$\Delta Gf° = -112.008 + 3.384 \times 10^{-3}T\ln T - 0.558 \times 10^{-6}T^{2} + 134.325T^{-1} - 8.582 \times 10^{-3}T$

Source: Data from JANAF (127) who estimated enthalpy of formation at 298 K.

$Al(OH)_3$(gibbsite)
Gibbsite

[Formation: $Al(c) + 1.5O_2(g) + 1.5H_2(g) = Al(OH)_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	21.924	16.358	16.358	0	-306.200	-273.184	200.247
300	22.043	16.494	16.358	.041	-306.209	-272.979	198.863
400	27.642	23.637	17.294	2.537	-306.417	-261.858	143.071
500	32.089	30.299	19.237	5.531	-306.192	-250.735	109.595
600	35.818	36.488	21.603	8.931	-305.626	-239.691	87.306
700	39.069	42.259	24.146	12.679	-304.780	-228.765	71.423

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 17.939 + 32.024 \times 10^{-3}T - 4.945 \times 10^{5}T^{-2}$

$H°-H°_{298} = 17.939 \times 10^{-3}T + 16.012 \times 10^{-6}T^{2} + 4.945 \times 10^{2}T^{-1} - 8.430$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -306.778 - 7.182 \times 10^{-3}T + 12.902 \times 10^{-6}T^{2} + 468.850T^{-1}$

$\Delta Gf° = -306.778 + 7.182 \times 10^{-3}T\ln T - 12.902 \times 10^{-6}T^{2} + 234.425T^{-1} + 72.964 \times 10^{-3}T$

Source: Enthalpy of formation at 298 K from Wagman (513). Other data from Haas (198).

$Al_2(SO_4)_3$(c)
Aluminum Sulfate
[Reaction: $2Al(c,l) + 1.5S_2(g) + 6O_2(g) = Al_2(SO_4)_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	62.000	57.200	57.200	0	-868.685	-769.657	564.167
300	62.140	57.584	57.201	.115	-868.691	-769.041	560.239
400	75.248	77.392	59.814	7.031	-868.428	-735.838	402.038
500	84.331	95.221	65.145	15.038	-867.295	-702.803	307.191
600	90.414	111.174	71.512	23.797	-865.641	-670.051	244.063
700	94.191	125.421	78.215	33.044	-863.717	-637.602	199.066
800	96.318	138.152	84.927	42.580	-861.714	-605.443	165.397
900	97.440	149.568	91.486	52.274	-859.744	-573.528	139.270
933.61	97.693	153.145	93.642	55.553	-859.100	-562.852	131.757
933.61	97.693	153.145	93.642	55.553	-864.260	-562.852	131.757
1000	98.194	159.874	97.818	62.056	-862.954	-541.465	118.335
1100	99.214	169.276	103.892	71.922	-860.982	-509.408	101.209

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 82.990 + 20.862 \times 10^{-3}T - 24.188 \times 10^{5}T^{-2}$

$H° - H°_{298} = 82.990 \times 10^{-3}T + 10.431 \times 10^{-6}T^{2} + 24.188 \times 10^{2}T^{-1} - 33.783$

Reaction equations (kcal/mol):

298.15-933.61 K: $\Delta Hr° = -881.311 + 17.911 \times 10^{-3}T + 3.479 \times 10^{-6}T^{2} + 2079.950T^{-1}$

$\Delta Gr° = -881.311 - 17.911 \times 10^{-3}T\ln T - 3.479 \times 10^{-6}T^{2} + 1039.975T^{-1} + 465.879 \times 10^{-3}T$

933.61-1100 K: $\Delta Hr° = -883.846 + 11.915 \times 10^{-3}T + 6.933 \times 10^{-6}T^{2} + 2045.150T^{-1}$

$\Delta Gr° = -883.846 - 11.915 \times 10^{-3}T\ln T - 6.933 \times 10^{-6}T^{2} + 1022.575T^{-1} + 430.832 \times 10^{-3}T$

Source: Data from DeKock (113).

$Al_2(SO_4)_3 \cdot 6H_2O(c)$
Aluminum Sulfate Hexahydrate
[Reaction: $2Al(c) + 1.5S_2(g) + 9O_2(g) + 6H_2(g) = Al_2(SO_4)_3 \cdot 6H_2O(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	118.061	112.188	112.188	0	-1315.835	-1133.543	830.899
300*	118.652	112.920	112.190	.219	-1315.854	-1132.411	824.950
350	133.954	132.376	113.693	6.539	-1315.967	-1101.821	687.999
400	147.974	151.193	117.210	13.593	-1315.427	-1071.256	585.300
450	160.712	169.369	122.000	21.316	-1314.295	-1040.794	505.472
500	172.166	186.906	127.620	29.643	-1312.639	-1010.489	441.679
550	182.338	203.803	133.783	38.511	-1310.516	-980.372	389.559

*Data above 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 79.742 + 199.648 \times 10^{-3}T - 18.851 \times 10^{5}T^{-2}$

$H° - H°_{298} = 79.742 \times 10^{-3}T + 99.824 \times 10^{-6}T^{2} + 18.851 \times 10^{2}T^{-1} - 38.971$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -1315.152 - 45.763 \times 10^{-3}T + 88.849 \times 10^{-6}T^{2} + 1509.650T^{-1}$

$\Delta Gr° = -1315.152 + 45.763 \times 10^{-3}T\ln T - 88.849 \times 10^{-6}T^{2} + 754.825T^{-1} + 366.383 \times 10^{-3}T$

Source: Data from DeKock (113) who estimated all above 298 K.

AlSb(c,l)
Aluminum Antimonide
[Formation: Al(c,l) + Sb(c,l) = AlSb(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.260	15.360	15.360	0	-12.200	-11.515	8.441
300	11.270	15.430	15.363	.020	-12.202	-11.511	8.386
400	11.680	18.760	15.810	1.180	-12.252	-11.272	6.159
500	11.890	21.390	16.670	2.360	-12.323	-11.017	4.815
600	12.090	23.580	17.647	3.560	-12.414	-10.752	3.916
700	12.300	25.450	18.621	4.780	-12.535	-10.455	3.264
800	12.500	27.110	19.585	6.020	-12.700	-10.156	2.774
900	12.700	28.590	20.501	7.280	-12.920	-9.820	2.385
903.9	12.708	28.645	20.536	7.330	-12.930	-9.806	2.371
903.9	12.708	28.645	20.536	7.330	-17.680	-9.806	2.371
933.61	12.771	29.057	20.801	7.708	-17.759	-9.544	2.234
933.61	12.771	29.057	20.801	7.708	-20.339	-9.544	2.234
1000	12.910	29.940	21.380	8.560	-20.489	-8.780	1.919
1100	13.110	31.180	22.216	9.860	-20.698	-7.595	1.509
1200	13.320	32.330	23.013	11.180	-20.887	-6.399	1.165
1300	13.520	33.410	23.779	12.520	-21.056	-5.196	.874
1330	13.590	33.720	23.998	12.930	-21.099	-4.827	.793
1330	17.800	48.450	23.999	32.520	-1.509	-4.827	.793
1400	17.800	49.360	25.239	33.770	-1.315	-4.993	.779
1500	17.800	50.590	26.890	35.550	-1.044	-5.265	.767

<u>Phase changes</u>: 903.9 K, melting point of Sb; $\Delta H^\circ = 4.750$ kcal/mol.
933.61 K, melting point of Al; $\Delta H^\circ = 2.580$ kcal/mol.
1330 K, melting point of AlSb; $\Delta H^\circ = 19.590$ kcal/mol.

<u>Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations</u>:

298.15-1330 K: $Cp^\circ = 11.272 + 1.688\times10^{-3}T - 0.458\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 11.272\times10^{-3}T + 0.844\times10^{-6}T^{2} + 0.458\times10^{2}T^{-1} - 3.589$
1330-1500 K: $Cp^\circ = 17.840$
$H^\circ - H^\circ_{298} = 17.840\times10^{-3}T + 8.793$

<u>Formation equations (kcal/mol)</u>:

298.15-903.9 K: $\Delta Hf^\circ = -12.776 + 1.592\times10^{-3}T - 2.055\times10^{-6}T^{2} + 84.800T^{-1}$
$\Delta Gf^\circ = -12.776 - 1.592\times10^{-3}T\ln T + 2.055\times10^{-6}T^{2} + 42.400T^{-1} + 12.210\times10^{-3}T$
903.9-933.61 K: $\Delta Hf^\circ = -16.280 - 0.820\times10^{-3}T - 0.883\times10^{-6}T^{2} + 63.200T^{-1}$
$\Delta Gf^\circ = -16.280 + 0.820\times10^{-3}T\ln T + 0.883\times10^{-6}T^{2} + 31.600T^{-1} + 0.741\times10^{-3}T$
933.61-1330 K: $\Delta Hf^\circ = -17.548 - 3.818\times10^{-3}T + 0.844\times10^{-6}T^{2} + 45.800T^{-1}$
$\Delta Gf^\circ = -17.548 + 3.818\times10^{-3}T\ln T - 0.844\times10^{-6}T^{2} + 22.900T^{-1} - 16.782\times10^{-3}T$
1330-1500 K: $\Delta Hf^\circ = -5.166 + 2.750\times10^{-3}T$
$\Delta Gf^\circ = -5.166 - 2.750\times10^{-3}T\ln T + 20.041\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Samokhval (<u>433</u>) and Sirota (<u>461</u>). Low-temperature heat capacities and entropy at 298 K from Piesbergen (<u>400</u>). High-temperature data based on Lichter (<u>308</u>).

$Al_4SiC_4(c)$
Tetraaluminum Silicon Tetracarbide
[Formation: $4Al(c,l) + Si(c,l) + 4C(c) = Al_4SiC_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	34.672	25.721	25.721	0	-48.590	-45.200	33.132
300	34.817	25.936	25.723	.064	-48.595	-45.180	32.913
400	40.077	36.732	27.157	3.830	-48.704	-44.024	24.053
500	43.534	46.070	30.030	8.020	-48.824	-42.841	18.726
600	46.060	54.240	33.397	12.506	-49.022	-41.620	15.160
700	48.041	61.495	36.904	17.214	-49.329	-40.367	12.603
800	49.670	68.019	40.391	22.102	-49.758	-39.056	10.670
900	51.057	73.952	43.795	27.141	-50.327	-37.693	9.153
933.61	51.465	75.831	44.915	28.864	-50.548	-37.216	8.712
933.61	51.465	75.831	44.915	28.864	-60.868	-37.216	8.712
1000	52.270	79.395	47.087	32.308	-61.216	-35.515	7.762
1100*	53.353	84.429	50.256	37.590	-61.703	-32.889	6.534
1200	54.338	89.114	53.301	42.975	-62.150	-30.290	5.516
1300	55.247	93.500	56.227	48.455	-62.556	-27.622	4.644
1400	56.098	97.625	59.037	54.023	-62.917	-24.914	3.889
1500	56.903	101.523	61.741	59.673	-63.238	-22.202	3.235
1600	57.677	105.221	64.344	65.403	-63.508	-19.455	2.657
1687	58.329	108.292	66.532	70.449	-63.714	-17.040	2.207
1687	58.329	108.292	66.532	70.449	-75.796	-17.040	2.207
1700	58.426	108.740	66.853	71.208	-75.814	-16.583	2.132
1800	59.161	112.100	69.274	77.087	-75.929	-13.087	1.589
1900	59.889	115.318	71.613	83.040	-75.990	-9.589	1.103
2000	60.616	118.409	73.876	89.065	-76.003	-6.101	.667

*Data extrapolated above 1047 K.

Phase changes: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 43.564 + 9.140x10^{-3}T - 10.327x10^{5}T^{-2}$
$H°- H°_{298} = 43.564x10^{-3}T + 4.570x10^{-6}T^{2} + 10.327x10^{2}T^{-1} - 16.859$

Formation equations (kcal/mol):

298.15-933.61 K: $ΔHf° = -50.757 + 5.445x10^{-3}T - 5.753x10^{-6}T^{2} + 314.600T^{-1}$
$ΔGf° = -50.757 - 5.445x10^{-3}TlnT + 5.753x10^{-6}T^{2} + 157.300T^{-1} + 46.178x10^{-3}T$
933.61-1687 K: $ΔHf° = -55.828 - 6.547x10^{-3}T + 1.155x10^{-6}T^{2} + 245.000T^{-1}$
$ΔGf° = -55.828 + 6.547x10^{-3}TlnT - 1.155x10^{-6}T^{2} + 122.500T^{-1} - 23.915x10^{-3}T$
1687-2000 K: $ΔHf° = -68.257 - 6.968x10^{-3}T + 1.506x10^{-6}T^{2} + 343.500T^{-1}$
$ΔGf° = -68.257 + 6.968x10^{-3}TlnT - 1.506x10^{-6}T^{2} + 171.750T^{-1} - 19.101x10^{-3}T$

Source: Data from Beyer (43) who extrapolated above 1047 K.

Al_2SiO_5(kyanite)
Aluminum Silicate, Kyanite
[Formation: $2Al(c,l) + Si(c) + 2.5O_2(g) = Al_2SiO_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	29.242	20.188	20.188	0	-620.000	-584.110	428.158
300	29.382	20.369	20.189	.054	-620.009	-583.887	425.356
400	35.339	29.706	21.421	3.314	-620.227	-571.804	312.415
500*	39.206	38.034	23.926	7.054	-620.109	-559.703	244.643
600	41.899	45.435	26.908	11.116	-619.808	-547.648	199.478
700	43.854	52.048	30.035	15.409	-619.416	-535.651	167.236
800	45.309	58.003	33.164	19.871	-618.992	-523.714	143.070
900	46.407	63.406	36.229	24.459	-618.578	-511.830	124.288
933.61	46.687	65.113	37.239	26.023	-618.446	-507.846	118.881
933.61	46.687	65.113	37.239	26.023	-623.606	-507.846	118.881
1000	47.241	68.341	39.198	29.143	-623.290	-499.618	109.190
1100	47.872	72.874	42.056	33.900	-622.785	-487.282	96.813
1200	48.343	77.061	44.801	38.712	-622.256	-474.986	86.506
1300	48.686	80.945	47.433	43.565	-621.711	-462.737	77.792
1400	48.923	84.562	49.958	48.446	-621.164	-450.523	70.329
1500	49.073	87.943	52.379	53.346	-620.620	-438.368	63.869
1600	49.149	91.113	54.702	58.258	-620.087	-426.237	58.220

*Metastable above 430 K.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 41.977 + 5.760\times10^{-3}T - 12.847\times10^{5}T^{-2}$
$H°-H°_{298} = 41.977\times10^{-3}T + 2.880\times10^{-6}T^{2} + 12.847\times10^{2}T^{-1} - 17.080$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -626.217 + 9.039\times10^{-3}T - 2.182\times10^{-6}T^{2} + 1108.000T^{-1}$
$\Delta Gf° = -626.217 - 9.039\times10^{-3}T\ln T + 2.182\times10^{-6}T^{2} + 554.000T^{-1} + 185.847\times10^{-3}T$
933.61-1600 K: $\Delta Hf° = -628.753 + 3.043\times10^{-3}T + 1.271\times10^{-6}T^{2} + 1073.200T^{-1}$
$\Delta Gf° = -628.753 - 3.043\times10^{-3}T\ln T - 1.271\times10^{-6}T^{2} + 536.600T^{-1} + 150.800\times10^{-3}T$

Source: Data from Haas (198).

Al_2SiO_5(andalusite)
Aluminum Silicate, Andalusite
[Formation: $2Al(c,l) + Si(c,l) + 2.5O_2(g) = Al_2SiO_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	29.157	22.413	22.413	0	-619.100	-583.873	427.985
300	29.296	22.593	22.413	.054	-619.109	-583.654	425.186
400	35.294	31.909	23.642	3.307	-619.334	-571.792	312.409
500*	39.075	40.223	26.145	7.039	-619.224	-559.912	244.734
600	41.506	47.578	29.116	11.077	-618.947	-548.073	199.633
700	43.121	54.106	32.229	15.314	-618.610	-536.286	167.434
800	44.249	59.941	35.335	19.685	-618.277	-524.550	143.299
900	45.102	65.204	38.366	24.154	-617.983	-512.853	124.536
933.61	45.345	66.862	39.362	25.674	-617.895	-508.928	119.134
933.61	45.345	66.862	39.362	25.674	-623.055	-508.928	119.134
1000	45.824	69.994	41.292	28.702	-622.831	-500.812	109.451
1100	46.512	74.394	44.105	33.318	-622.467	-488.636	97.082
1200	47.240	78.472	46.801	38.005	-622.063	-476.486	86.779
1300	48.059	82.285	49.386	42.769	-621.607	-464.375	78.067
1400	49.011	85.880	51.865	47.621	-621.089	-452.294	70.605
1500	50.125	89.298	54.247	52.577	-620.489	-440.270	64.146
1600	51.425	92.574	56.541	57.653	-619.792	-428.279	58.499
1687	52.736	95.330	58.471	62.182	-619.087	-417.862	54.133
1687	52.736	95.330	58.471	62.182	-631.169	-417.862	54.133
1700	52.932	95.736	58.754	62.869	-631.046	-416.215	53.507
1800	54.661	98.809	60.895	68.246	-630.017	-403.602	49.003

*Metastable below 430 K and above 1017 K.

Phase changes: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 39.629 + 7.550\times10^{-3}T - 11.310\times10^{5}T^{-2}$
$H°-H°_{298} = 39.629\times10^{-3}T + 3.775\times10^{-6}T^{2} + 11.310\times10^{2}T^{-1} - 15.944$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -624.181 + 6.691\times10^{-3}T - 1.287\times10^{-6}T^{2} + 954.300T^{-1}$
$\Delta Gf° = -624.181 - 6.691\times10^{-3}T\ln T + 1.287\times10^{-6}T^{2} + 477.150T^{-1} + 167.565\times10^{-3}T$
933.61-1687 K: $\Delta Hf° = -626.717 + 0.695\times10^{-3}T + 2.167\times10^{-6}T^{2} + 919.500T^{-1}$
$\Delta Gf° = -626.717 - 0.695\times10^{-3}T\ln T - 2.167\times10^{-6}T^{2} + 459.750T^{-1} + 132.518\times10^{-3}T$
1687-1800 K: $\Delta Hf° = -639.146 + 0.274\times10^{-3}T + 2.518\times10^{-6}T^{2} + 1018.000T^{-1}$
$\Delta Gf° = -639.146 - 0.274\times10^{-3}T\ln T - 2.518\times10^{-6}T^{2} + 509.000T^{-1} + 137.333\times10^{-3}T$

Source: Data from Haas (198).

Al_2SiO_5(sillimanite)
Aluminum Silicate, Sillimanite
[Formation: $2Al(c,l) + Si(c,l) + 2.5O_2(g) = Al_2SiO_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	29.764	22.966	22.966	0	-618.500	-583.438	427.666
300	29.891	23.151	22.968	.055	-618.508	-583.221	424.871
400	35.289	32.550	24.212	3.335	-618.706	-571.420	312.206
500	38.830	40.829	26.725	7.052	-618.611	-559.602	244.599
600	41.324	48.141	29.696	11.067	-618.357	-547.821	199.541
700	43.162	54.656	32.806	15.295	-618.030	-536.090	167.373
800	44.556	60.515	35.910	19.684	-617.678	-524.410	143.260
900	45.633	65.828	38.944	24.196	-617.341	-512.773	124.517
933.61	45.916	67.506	39.942	25.734	-617.235	-508.869	119.120
933.61	45.916	67.506	39.942	25.734	-622.395	-508.869	119.120
1000	46.474	70.681	41.878	28.803	-622.130	-500.798	109.448
1100*	47.134	75.143	44.702	33.485	-621.701	-488.693	97.093
1200	47.653	79.267	47.413	38.225	-621.243	-476.620	86.803
1300	48.057	83.098	50.012	43.012	-620.763	-464.589	78.103
1400	48.367	86.671	52.505	47.833	-620.277	-452.589	70.651
1500	48.600	90.017	54.896	52.682	-619.784	-440.643	64.201
1600	48.767	93.159	57.190	57.551	-619.294	-428.717	58.559
1687	48.864	95.744	59.112	61.799	-618.870	-418.344	54.196
1687	48.864	95.744	59.112	61.799	-630.952	-418.344	54.196
1700	48.879	96.119	59.393	62.434	-630.881	-416.701	53.570
1800	48.943	98.915	61.512	67.326	-630.337	-404.113	49.065

*Metastable below 1017 K.

Phase changes: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1687.00 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp^\circ = 41.851 + 4.980\times10^{-3}T - 12.060\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 41.851\times10^{-3}T + 2.490\times10^{-6}T^{2} + 12.060\times10^{2}T^{-1} - 16.744$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -624.381 + 8.913\times10^{-3}T - 2.572\times10^{-6}T^{2} + 1029.300T^{-1}$
$\Delta Gf^\circ = -624.381 - 8.913\times10^{-3}T\ln T + 2.572\times10^{-6}T^{2} + 514.650T^{-1} + 181.550\times10^{-3}T$
933.61-1687 K: $\Delta Hf^\circ = -626.916 + 2.917\times10^{-3}T + 0.882\times10^{-6}T^{2} + 994.500T^{-1}$
$\Delta Gf^\circ = -626.916 - 2.917\times10^{-3}T\ln T - 0.882\times10^{-6}T^{2} + 497.250T^{-1} + 146.503\times10^{-3}T$
1687-1800 K: $\Delta Hf^\circ = -639.345 + 2.496\times10^{-3}T + 1.233\times10^{-6}T^{2} + 1093.000T^{-1}$
$\Delta Gf^\circ = -639.345 - 2.496\times10^{-3}T\ln T - 1.233\times10^{-6}T^{2} + 546.500T^{-1} + 151.317\times10^{-3}T$

Source: Data from Haas (198).

$Al_6Si_2O_{13}$(mullite)
Trialumino Disilicate, Mullite
[Formation: $6Al(c,l) + 2Si(c,l) + 6.5O_2(g) = Al_6Si_2O_{13}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	77.830	65.700	65.700	0	-1632.800	-1542.613	1130.751
300	78.162	66.183	65.703	.144	-1632.824	-1542.054	1123.371
400	93.390	90.882	68.965	8.767	-1633.419	-1511.681	825.934
500	103.250	112.840	75.590	18.625	-1633.148	-1481.259	647.449
600	109.900	132.283	83.451	29.299	-1632.432	-1450.939	528.497
700	114.600	149.592	91.686	40.534	-1631.527	-1420.759	443.575
800	118.100	165.134	99.913	52.177	-1630.596	-1390.719	379.922
900	120.650	179.196	107.953	64.119	-1629.745	-1360.787	330.440
933.61	121.339	183.632	110.598	68.186	-1629.487	-1350.746	316.194
933.61	121.339	183.632	110.598	68.186	-1644.967	-1350.746	316.194
1000	122.700	192.016	115.728	76.288	-1644.307	-1329.834	290.631
1100	124.212	203.782	123.205	88.635	-1643.242	-1298.452	257.975
1200	125.626	214.652	130.380	101.127	-1642.104	-1267.154	230.777
1300	126.940	224.760	137.255	113.757	-1640.892	-1235.962	207.781
1400	128.154	234.212	143.846	126.512	-1639.621	-1204.850	188.083
1500	129.270	243.092	150.169	139.384	-1638.284	-1173.871	171.031
1600	130.097	251.461	156.241	152.352	-1636.906	-1142.956	156.119
1687	130.812	258.368	161.331	163.702	-1635.676	-1116.087	144.587
1687	130.812	258.368	161.331	163.702	-1659.840	-1116.087	144.587
1700	130.919	259.373	162.077	165.403	-1659.636	-1111.889	142.941
1800	131.737	266.880	167.693	178.536	-1658.049	-1079.704	131.092
1900	132.551	274.024	173.102	191.751	-1656.419	-1047.613	120.501
2000	133.360	280.844	178.321	205.046	-1654.742	-1015.631	110.982

Phase changes: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 111.991 + 12.298\times10^{-3}T - 33.627\times10^{5}T^{-2}$
$H°-H°_{298} = 111.991\times10^{-3}T + 6.149\times10^{-6}T^{2} + 33.627\times10^{2}T^{-1} - 45.215$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -1649.833 + 26.086\times10^{-3}T - 8.184\times10^{-6}T^{2} + 2976.300T^{-1}$
$\Delta Gf° = -1649.833 - 26.086\times10^{-3}T\ln T + 8.184\times10^{-6}T^{2} + 1488.150T^{-1} + 489.062\times10^{-3}T$
933.61-1687 K: $\Delta Hf° = -1657.439 + 8.098\times10^{-3}T + 2.178\times10^{-6}T^{2} + 2871.900T^{-1}$
$\Delta Gf° = -1657.439 - 8.098\times10^{-3}T\ln T - 2.178\times10^{-6}T^{2} + 1435.950T^{-1} + 383.922\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -1682.297 + 7.256\times10^{-3}T + 2.880\times10^{-6}T^{2} + 3068.900T^{-1}$
$\Delta Gf° = -1682.297 - 7.256\times10^{-3}T\ln T - 2.880\times10^{-6}T^{2} + 1534.450T^{-1} + 393.550\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data from JANAF (127).

$Al_2TiO_5(c)$
Aluminum Titanate
[Formation: $2Al(c,l) + Ti(c) + 2.5O_2(g) = Al_2TiO_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	32.604	26.200	26.200	0	-620.600	-585.661	429.296
300	32.772	26.402	26.202	.060	-620.605	-585.444	426.490
400	38.857	36.779	27.574	3.682	-620.570	-573.716	313.460
500	41.940	45.812	30.340	7.736	-620.235	-562.038	245.663
600	43.841	53.639	33.587	12.031	-619.793	-550.437	200.494
700	45.185	60.503	36.952	16.486	-619.336	-538.907	168.252
800	46.232	66.607	40.283	21.059	-618.909	-527.451	144.091
900	47.106	72.104	43.518	25.727	-618.534	-516.041	125.310
933.61	47.363	73.836	44.579	27.315	-618.421	-512.216	119.904
933.61	47.363	73.836	44.579	27.315	-623.581	-512.216	119.904
1000	47.872	77.108	46.632	30.476	-623.311	-504.306	110.215
1100	48.569	81.704	49.614	35.299	-622.886	-492.432	97.836
1156	48.932	84.125	51.227	38.030	-622.638	-485.791	91.841
1156	48.932	84.125	51.227	38.030	-623.655	-485.791	91.841
1200	49.217	85.958	52.467	40.189	-623.409	-480.548	87.519
1300	49.832	89.922	55.198	45.141	-622.836	-468.669	78.789
1400	50.423	93.637	57.813	50.154	-622.242	-456.832	71.314
1500	50.995	97.135	60.318	55.225	-621.625	-445.039	64.841
1600	51.554	100.444	62.723	60.353	-620.989	-433.287	59.184
1700	52.102	103.586	65.035	65.536	-620.335	-421.574	54.196
1800	52.642	106.579	67.261	70.773	-619.672	-409.900	49.768

Phase changes: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1156 K, α - β transition of Ti; ΔH° = 1.017 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 44.053 + 4.968\times10^{-3}T - 11.495\times10^{5}T^{-2}$
$H°-H°_{298} = 44.053\times10^{-3}T + 2.484\times10^{-6}T^{2} + 11.495\times10^{2}T^{-1} - 17.211$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -627.220 + 11.317\times10^{-3}T - 3.351\times10^{-6}T^{2} + 1056.500T^{-1}$
$\Delta Gf° = -627.220 - 11.317\times10^{-3}T\ln T + 3.351\times10^{-6}T^{2} + 528.250T^{-1} + 196.926\times10^{-3}T$
933.61-1156 K: $\Delta Hf° = -629.755 + 5.321\times10^{-3}T + 0.104\times10^{-6}T^{2} + 1021.700T^{-1}$
$\Delta Gf° = -629.755 - 5.321\times10^{-3}T\ln T - 0.104\times10^{-6}T^{2} + 510.850T^{-1} + 161.879\times10^{-3}T$
1156-1800 K: $\Delta Hf° = -633.792 + 7.721\times10^{-3}T - 0.219\times10^{-6}T^{2} + 1804.600T^{-1}$
$\Delta Gf° = -633.792 - 7.721\times10^{-3}T\ln T + 0.219\times10^{-6}T^{2} + 902.300T^{-1} + 181.631\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Gani (169). Low-temperature heat capacities and entropy at 298 K from King (259). High-temperature data based on Bonnickson (52).

$AsH_3(g)$
Arsenic Trihydride (ideal gas)
[Formation: $As[\alpha, 1/4As_4(g)] + 1.5H_2(g) = AsH_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	9.100	53.220	53.220	0	15.880	16.513	-12.105
300	9.120	53.270	53.220	.020	15.870	16.522	-12.036
400	10.320	56.060	53.585	.990	15.199	16.841	-9.201
500	11.480	58.490	54.330	2.080	14.627	17.319	-7.570
600	12.550	60.680	55.205	3.285	14.155	17.904	-6.522
700	13.510	62.690	56.133	4.590	13.767	18.561	-5.795
800	14.360	64.550	57.069	5.985	13.450	19.270	-5.264
876	14.907	65.875	57.781	7.090	13.240	19.825	-4.946
876	14.907	65.875	57.781	7.090	4.931	19.825	-4.946
900	15.080	66.280	58.002	7.450	4.917	20.234	-4.913
1000	15.690	67.900	58.910	8.990	4.887	21.939	-4.795

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol of $As_4(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 7.226 + 9.058 \times 10^{-3}T - 0.735 \times 10^{5}T^{-2}$
$H° - H°_{298} = 7.226 \times 10^{-3}T + 4.529 \times 10^{-6}T^{2} + 0.735 \times 10^{2}T^{-1} - 2.804$

Formation equations (kcal/mol):

298.15-876 K: $\Delta Hf° = 17.726 - 8.149 \times 10^{-3}T + 3.329 \times 10^{-6}T^{2} + 85.850T^{-1}$
$\Delta Gf° = 17.726 + 8.149 \times 10^{-3}T\ln T - 3.329 \times 10^{-6}T^{2} + 42.925T^{-1} - 49.986 \times 10^{-3}T$
876-1000 K: $\Delta Hf° = 8.398 - 7.451 \times 10^{-3}T + 3.907 \times 10^{-6}T^{2} + 54.350T^{-1}$
$\Delta Gf° = 8.398 + 7.451 \times 10^{-3}T\ln T - 3.907 \times 10^{-6}T^{2} + 27.175T^{-1} - 34.081 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data from Sundaram (486).

AsSe(g)
Arsenic Selenide (ideal gas)
[Reaction: $As[\alpha, 1/4As_4(g)] + 0.5Se_2(g) = AsSe(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	8.540	59.190	59.190	0	32.850	26.423	-19.368
300	8.540	59.240	59.190	.016	32.846	26.384	-19.220
400	8.580	61.700	59.520	.872	32.605	24.267	-13.258
500	8.620	63.620	60.156	1.732	32.347	22.212	-9.709
600	8.650	65.200	60.875	2.595	32.078	20.205	-7.359
700	8.690	66.530	61.584	3.462	31.800	18.253	-5.699
800	8.730	67.700	62.284	4.333	31.514	16.333	-4.462
876	8.753	68.493	62.788	4.998	31.292	14.899	-3.717
876	8.753	68.493	62.788	4.998	22.983	14.899	-3.717
900	8.760	68.730	62.943	5.208	22.955	14.678	-3.564
1000	8.800	69.650	63.564	6.086	22.840	13.767	-3.009
1100	8.840	70.490	64.155	6.968	22.731	12.868	-2.557
1200	8.880	71.260	64.715	7.854	22.630	11.977	-2.181
1300	8.910	71.980	65.255	8.743	22.532	11.084	-1.863
1400	8.950	72.640	65.756	9.637	22.443	10.208	-1.594
1500	8.990	73.260	66.237	10.534	22.359	9.336	-1.360
1600	9.020	73.840	66.694	11.434	22.282	8.469	-1.157

*Data estimated.

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol of $As_4(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.430 + 0.372\text{x}10^{-3}T$

$H^\circ - H^\circ_{298} = 8.430\text{x}10^{-3}T + 0.186\text{x}10^{-6}T^2 - 2.530$

Reaction equations (kcal/mol):

298.15-876 K: $\Delta Hr^\circ = 33.785 - 2.593\text{x}10^{-3}T - 0.225\text{x}10^{-6}T^2 - 42.350T^{-1}$

$\Delta Gr^\circ = 33.785 + 2.593\text{x}10^{-3}T\ln T + 0.225\text{x}10^{-6}T^2 - 21.175T^{-1} - 39.296\text{x}10^{-3}T$

876-1600 K: $\Delta Hr^\circ = 24.457 - 1.895\text{x}10^{-3}T + 0.353\text{x}10^{-6}T^2 - 73.850T^{-1}$

$\Delta Gr^\circ = 24.457 + 1.895\text{x}10^{-3}T\ln T - 0.353\text{x}10^{-6}T^2 - 36.925T^{-1} - 23.391\text{x}10^{-3}T$

Source: Data are those estimated by Mills (332).

As_2Se_3(c,l)
Diarsenic Triselenide (ideal gas)
[Reaction: $2As(\alpha) + 1.5Se_2(g) = As_2Se_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	29.050	46.500	46.500	0	-74.450	-57.197	41.926
300	29.077	46.680	46.500	.054	-74.445	-57.090	41.590
400	30.346	55.227	47.657	3.028	-74.164	-51.346	28.054
500	32.011	62.162	49.884	6.139	-73.791	-45.680	19.966
600	34.650	68.215	52.443	9.463	-73.237	-40.110	14.610
634	35.807	70.156	53.342	10.660	-72.988	-38.240	13.182
634	51.677	74.888	53.342	13.660	-69.988	-38.240	13.182
700	53.891	80.093	55.622	17.130	-68.365	-35.013	10.931
800	60.934	87.709	59.157	22.842	-65.471	-30.432	8.313

Phase change: 634 K, melting point of As_2Se_3; ΔH° = 3.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-634 K: $Cp° = 18.513 + 25.384\times10^{-3}T + 2.637\times10^{5}T^{-2}$

$H°- H°_{298} = 18.513\times10^{-3}T + 12.692\times10^{-6}T^{2} - 2.637\times10^{2}T^{-1} - 5.763$

634-800 K: $Cp° = 16.058 + 54.750\times10^{-3}T$

$H°- H°_{298} = 16.058\times10^{-3}T + 27.375\times10^{-6}T^{2} - 7.524$

Reaction equations (kcal/mol):

298.15-634 K: $\Delta Hr° = -71.607 - 8.865\times10^{-3}T + 12.028\times10^{-6}T^{2} - 378.350T^{-1}$

$\Delta Gr° = -71.607 + 8.865\times10^{-3}T\ln T - 12.028\times10^{-6}T^{2} - 189.175T^{-1} + 3.538\times10^{-3}T$

634-800 K: $\Delta Hr° = -73.369 - 11.320\times10^{-3}T + 26.712\times10^{-6}T^{2} - 114.650T^{-1}$

$\Delta Gr° = -73.369 + 11.320\times10^{-3}T\ln T - 26.712\times10^{-6}T^{2} - 57.325T^{-1} - 0.542\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (332). Low-temperature heat capacities and entropy at 298 K from Zhdanov (545). High-temperature data based on Rasulov (415).

AsTe(g)
Arsenic Telluride (ideal gas)
[Reaction: $As[\alpha,1/4As_4(g)] + 0.5Te_2(g) = AsTe(g)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	8.750	61.090	61.090	.0	35.535	29.089	-21.322
300	8.750	61.140	61.090	.016	35.532	29.049	-21.162
400	8.770	63.660	61.430	.892	35.368	26.913	-14.704
500	8.780	65.620	62.082	1.769	35.185	24.819	-10.848
600	8.800	67.220	62.807	2.648	34.980	22.768	-8.293
700	8.820	68.580	63.539	3.529	34.757	20.747	-6.478
800	8.830	69.760	64.245	4.412	34.514	18.761	-5.125
876	8.845	70.561	64.758	5.084	34.316	17.272	-4.309
876	8.845	70.561	64.758	5.084	26.007	17.272	-4.309
900	8.850	70.800	64.916	5.296	25.985	17.033	-4.136
1000	8.870	71.730	65.548	6.182	25.889	16.046	-3.507
1100	8.880	72.580	66.153	7.070	25.786	15.065	-2.993
1200	8.900	73.350	66.717	7.959	25.676	14.100	-2.568
1300	8.920	74.070	67.262	8.850	25.560	13.131	-2.207
1400	8.940	74.730	67.771	9.743	25.438	12.181	-1.901
1500	8.950	75.350	68.259	10.637	25.314	11.234	-1.637
1600	8.970	75.920	68.712	11.533	25.193	10.308	-1.408

*Data estimated.

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; $\Delta H^\circ = 33.235$ kcal/mol of $As_4(g)$.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.698 + 0.170\times10^{-3}T$
$H^\circ - H^\circ_{298} = 8.698\times10^{-3}T + 0.085\times10^{-6}T^2 - 2.601$

Reaction equations (kcal/mol):

298.15-876 K: $\Delta Hr^\circ = 36.072 - 1.293\times10^{-3}T - 0.782\times10^{-6}T^2 - 24.500T^{-1}$
$\Delta Gr^\circ = 36.072 + 1.293\times10^{-3}T\ln T + 0.782\times10^{-6}T^2 - 12.250T^{-1} - 30.882\times10^{-3}T$
876-1600 K: $\Delta Hr^\circ = 26.744 - 0.595\times10^{-3}T - 0.204\times10^{-6}T^2 - 56.000T^{-1}$
$\Delta Gr^\circ = 26.744 + 0.595\times10^{-3}T\ln T + 0.204\times10^{-6}T^2 - 28.000T^{-1} - 14.978\times10^{-3}T$

Source: Data are those estimated by Mills (332).

$As_2Te_3(c,l)$
Diarsenic Tritelluride

[Reaction: $2As[\alpha, 1/4As_4(g)] + 1.5Te_2(g) = As_2Te_3(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H^\circ_{298})/T$	$H°-H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	30.470	54.100	54.100	0	-66.495	-49.866	36.552
300	30.564	54.289	54.102	.056	-66.485	-49.766	36.254
358	38.407	60.222	54.607	2.010	-65.987	-46.570	28.430
358	26.571	60.222	54.607	2.010	-65.987	-46.570	28.430
400	29.588	63.350	55.362	3.195	-65.865	-44.299	24.203
500	33.286	70.385	57.675	6.355	-65.275	-38.966	17.032
600	37.808	76.810	60.335	9.885	-64.368	-33.779	12.304
655	41.855	80.291	61.863	12.070	-63.647	-31.007	10.346
655	69.000	99.100	61.863	24.390	-51.327	-31.007	10.346
700	69.000	103.685	64.406	27.495	-49.432	-29.675	9.265
800	69.000	112.898	69.904	34.395	-45.257	-27.141	7.414
876	69.000	119.160	73.910	39.639	-42.115	-25.570	6.379
876	69.000	119.160	73.910	39.639	-58.733	-25.570	6.379
900	69.000	121.025	75.142	41.295	-57.662	-24.676	5.992

Phase changes: 358 K, α - β transition point of As_2Te_3 ΔH° = 0 kcal/mol.
655 K, melting point of As_2Te_3 ΔH° = 12.320 kcal/mol.
876 K, sublimation point of As(c) to As_4(g); ΔH° = 33.235 kcal/mol of As_4(g).

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-358 K: $Cp° = 33.449 + 48.740\times10^{-3}T - 16.923\times10^{5}T^{-2}$
$H°-H^\circ_{298} = 33.449\times10^{-3}T + 24.370\times10^{-6}T^2 + 16.923\times10^{2}T^{-1} - 17.815$
358-655 K: $Cp° = 25.690 + 24.774\times10^{-3}T - 10.238\times10^{5}T^{-2}$
$H°-H^\circ_{298} = 25.690\times10^{-3}T + 12.387\times10^{-6}T^2 + 10.238\times10^{2}T^{-1} - 11.634$
655-900 K: $Cp° = 69.000$
$H°-H^\circ_{298} = 69.000\times10^{-3}T - 20.805$

Reaction equations (kcal/mol):

298.15-358 K: $\Delta Hr° = -76.685 + 9.169\times10^{-3}T + 22.338\times10^{-6}T^2 + 1631.200T^{-1}$
$\Delta Gr° = -76.685 - 9.169\times10^{-3}T\ln T - 22.338\times10^{-6}T^2 + 815.600T^{-1} + 139.675\times10^{-3}T$
358-655 K: $\Delta Hr° = -70.505 + 1.410\times10^{-3}T + 10.356\times10^{-6}T^2 + 962.700T^{-1}$
$\Delta Gr° = -70.505 - 1.410\times10^{-3}T\ln T - 10.356\times10^{-6}T^2 + 481.350T^{-1} + 75.102\times10^{-3}T$
655-876 K: $\Delta Hr° = -79.675 + 44.719\times10^{-3}T - 2.031\times10^{-6}T^2 - 61.100T^{-1}$
$\Delta Gr° = -79.675 - 44.719\times10^{-3}T\ln T + 2.031\times10^{-6}T^2 - 30.550T^{-1} + 363.032\times10^{-3}T$
876-900 K: $\Delta Hr° = -98.331 + 46.115\times10^{-3}T - 0.875\times10^{-6}T^2 - 124.100T^{-1}$
$\Delta Gr° = -98.331 - 46.115\times10^{-3}T\ln T + 0.875\times10^{-6}T^2 - 62.050T^{-1} + 394.841\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (332). Low-temperature heat capacities and entropy at 298 K from Zhdanov (545). High-temperature data based on Medzhidov (329).

AuO(g)
Gold Oxide (ideal gas)
[Formation: $Au(c,l) + 0.5O_2(g) = AuO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	8.700	60.203	60.203	0	94.500	87.234	-63.943
300	8.710	60.256	60.203	.016	94.498	87.189	-63.517
400	8.810	62.779	60.547	.893	94.406	84.766	-46.313
500	8.860	64.749	61.197	1.776	94.301	82.369	-36.003
600	8.880	66.366	61.928	2.663	94.176	79.993	-29.137
700	8.900	67.736	62.662	3.552	94.031	77.641	-24.240
800	8.910	68.925	63.373	4.442	93.867	75.310	-20.573
900	8.910	69.975	64.049	5.333	93.688	73.001	-17.727
1000	8.920	70.914	64.689	6.225	93.496	70.713	-15.454
1100	8.920	71.765	65.295	7.117	93.287	68.444	-13.598
1200	8.930	72.542	65.867	8.010	93.050	66.196	-12.056
1300	8.930	73.256	66.408	8.902	92.758	63.968	-10.754
1337.58	8.930	73.510	66.604	9.238	92.627	63.137	-10.316
1337.58	8.930	73.510	66.604	9.238	89.670	63.137	-10.316
1400	8.930	73.918	66.921	9.796	89.460	61.905	-9.664
1500	8.930	74.534	67.409	10.688	89.121	59.948	-8.734
1600	8.930	75.110	67.872	11.581	88.778	58.014	-7.924
1700	8.930	75.652	68.314	12.475	88.434	56.103	-7.212
1800	8.930	76.163	68.736	13.368	88.086	54.210	-6.582
1900	8.930	76.646	69.140	14.262	87.735	52.337	-6.020
2000	8.940	77.105	69.528	15.155	87.382	50.481	-5.516

Phase change: 1337.58 K, melting point of Au; ΔH° = 2.957 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.940 - 0.210\times10^{5}T^{-2}$
$H° - H°_{298} = 8.940\times10^{-3}T + 0.210\times10^{2}T^{-1} - 2.736$

Formation equations (kcal/mol):

298.15-1337.58 K: $\Delta Hf° = 94.557 - 0.084\times10^{-3}T - 1.012\times10^{-6}T^{2} + 17.200T^{-1}$
$\Delta Gf° = 94.557 + 0.084\times10^{-3}T\ln T + 1.012\times10^{-6}T^{2} + 8.600T^{-1} - 25.440\times10^{-3}T$
1337.58-2000 K: $\Delta Hf° = 93.683 - 2.647\times10^{-3}T - 0.251\times10^{-6}T^{2} - 1.600T^{-1}$
$\Delta Gf° = 93.683 + 2.647\times10^{-3}T\ln T + 0.251\times10^{-6}T^{2} - 0.800T^{-1} - 42.214\times10^{-3}T$

Source: Data from Pedley (396).

AuSe(α)
α-Gold Selenide
[Reaction: Au(c) + $0.5Se_2(g)$ = AuSe(c)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	11.990	18.100	18.100	0	-19.950	-13.292	9.743
300	12.000	18.170	18.100	.022	-19.948	-13.250	9.652
400	12.670	21.720	18.580	1.256	-19.826	-11.036	6.030
500	13.330	24.620	19.508	2.556	-19.652	-8.858	3.872
600	14.000	27.110	20.572	3.923	-19.425	-6.721	2.448
700	14.670	29.310	21.659	5.356	-19.143	-4.619	1.442

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 10.000 + 6.670\times10^{-3}T$

$H°- H°_{298} = 10.000\times10^{-3}T + 3.335\times10^{-6}T^2 - 3.278$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta Hr° = -19.935 - 0.741\times10^{-3}T + 2.734\times10^{-6}T^2 - 11.150T^{-1}$

$\Delta Gr° = -19.935 + 0.741\times10^{-3}T\ln T - 2.734\times10^{-6}T^2 - 5.575T^{-1} + 18.935\times10^{-3}T$

Source: Data are those estimated by Mills (332).

$AuTe_2$(c)
Gold Ditelluride
[Reaction: $Au(c) + Te_2(g) = AuTe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^o_{298})/T$	$H°- H^o_{298}$	ΔHf°	ΔGf°	
298.15	18.330	33.870	33.870	0	-42.780	-31.054	22.763
300	18.340	33.980	33.870	.034	-42.773	-30.981	22.569
400	19.030	39.360	34.603	1.903	-42.397	-27.108	14.811
500	19.830	43.690	36.000	3.845	-41.974	-23.332	10.198
600	20.670	47.380	37.597	5.870	-41.496	-19.645	7.155
700	21.540	50.630	39.229	7.981	-40.960	-16.044	5.009
737	21.860	51.740	39.827	8.780	-40.750	-14.731	4.368

Phase change: 737 K, melting point of $AuTe_2$; ΔH° = 9.7 ± 3 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-737 K: $Cp° = 15.510 + 8.454\times10^{-3}T + 0.266\times10^{5}T^{-2}$

$H°- H^o_{298} = 15.510\times10^{-3}T + 4.227\times10^{-6}T^{2} - 0.266\times10^{2}T^{-1} - 4.911$

Reaction equations (kcal/mol):

298.15-737 K: $\Delta Hr° = -43.376 + 1.502\times10^{-3}T + 2.874\times10^{-6}T^{2} - 32.000T^{-1}$

$\Delta Gr° = -43.376 - 1.502\times10^{-3}T\ln T - 2.874\times10^{-6}T^{2} - 16.000T^{-1} + 50.924\times10^{-3}T$

Source: Data from Mills (332).

BC(g)
Boron Carbide (ideal gas)
[Formation: $B(\beta,l) + C(c) = BC(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.099	49.822	49.822	0	198.000	183.975	-134.856
300	7.102	49.866	49.823	.013	198.004	183.889	-133.961
400	7.359	51.942	50.102	.736	198.166	179.154	-97.884
500	7.642	53.615	50.643	1.486	198.192	174.398	-76.228
600	7.895	55.031	51.259	2.263	198.117	169.643	-61.792
700	8.102	56.265	51.889	3.063	197.975	164.908	-51.486
800	8.267	57.358	52.506	3.882	197.789	160.198	-43.763
900	8.398	58.339	53.100	4.715	197.566	155.511	-37.763
1000	8.504	59.230	53.669	5.561	197.317	150.852	-32.968
1100	8.589	60.044	54.211	6.416	197.044	146.224	-29.052
1200	8.659	60.795	54.730	7.278	196.749	141.607	-25.790
1300	8.717	61.490	55.223	8.147	196.434	137.028	-23.036
1400	8.766	62.138	55.694	9.021	196.101	132.470	-20.679
1500	8.809	62.744	56.144	9.900	195.749	127.941	-18.641
1600	8.845	63.314	56.575	10.783	195.380	123.422	-16.858
1700	8.877	63.851	56.987	11.669	194.992	118.936	-15.290
1800	8.906	64.360	57.383	12.558	194.588	114.484	-13.900
1900	8.932	64.842	57.763	13.450	194.168	110.047	-12.658
2000	8.955	65.300	58.128	14.344	193.730	105.620	-11.541
2100	8.976	65.738	58.480	15.241	193.277	101.234	-10.535
2200	8.996	66.156	58.820	16.139	192.807	96.852	-9.621
2300	9.014	66.556	59.147	17.040	192.322	92.516	-8.791
2350	9.023	66.750	59.307	17.491	192.072	90.330	-8.401
2350	9.023	66.750	59.307	17.491	180.072	90.330	-8.401
2400	9.031	66.940	59.464	17.942	179.841	88.432	-8.053
2500	9.047	67.309	59.771	18.846	179.378	84.618	-7.397

Phase change: 2350 K, melting point of B; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp^\circ = 7.792 + 0.642\times10^{-3}T - 0.786\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.792\times10^{-3}T + 0.321\times10^{-6}T^{2} + 0.786\times10^{2}T^{-1} - 2.615$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 199.292 - 0.449\times10^{-3}T - 1.137\times10^{-6}T^{2} - 315.200T^{-1}$

$\Delta Gf^\circ = 199.292 + 0.449\times10^{-3}T\ln T + 1.137\times10^{-6}T^{2} - 157.600T^{-1} - 52.498\times10^{-3}T$

2000-2350 K: $\Delta Hf^\circ = 201.284 - 2.572\times10^{-3}T - 0.505\times10^{-6}T^{2} - 862.900T^{-1}$

$\Delta Gf^\circ = 201.284 + 2.572\times10^{-3}T\ln T + 0.505\times10^{-6}T^{2} - 431.450T^{-1} - 68.298\times10^{-3}T$

2350-2500 K: $\Delta Hf^\circ = 191.894 - 5.349\times10^{-3}T + 0.187\times10^{-6}T^{2} - 641.400T^{-1}$

$\Delta Gf^\circ = 191.894 + 5.349\times10^{-3}T\ln T - 0.187\times10^{-6}T^{2} - 320.700T^{-1} - 84.252\times10^{-3}T$

Source: Data from JANAF (127).

$BC_2(g)$
Boron Dicarbide (ideal gas)
[Formation: $B(\beta) + 2C(c) = BC_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	10.927	56.542	56.542	0	189.000	173.381	-127.090
300	10.937	56.609	56.542	.020	189.007	173.284	-126.236
400	11.458	59.827	56.977	1.140	189.322	167.990	-91.784
500	11.947	62.438	57.816	2.311	189.452	162.640	-71.089
600	12.385	64.656	58.776	3.528	189.440	157.275	-57.287
700	12.763	66.594	59.757	4.786	189.332	151.923	-47.432
800	13.081	68.320	60.722	6.078	189.160	146.590	-40.046
900	13.344	69.876	61.654	7.400	188.939	141.280	-34.307
1000	13.561	71.293	62.547	8.746	188.683	136.000	-29.722
1100	13.741	72.595	63.403	10.111	188.396	130.759	-25.979
1200	13.890	73.797	64.219	11.493	188.083	125.514	-22.859
1300	14.014	74.914	65.000	12.888	187.744	120.316	-20.227
1400	14.119	75.956	65.745	14.295	187.385	115.142	-17.974
1500	14.208	76.934	66.459	15.712	187.003	109.999	-16.027
1600	14.284	77.853	67.143	17.136	186.601	104.868	-14.324
1700	14.351	78.721	67.799	18.568	186.177	99.771	-12.826
1800	14.411	79.543	68.429	20.006	185.735	94.714	-11.500
1900	14.466	80.324	69.035	21.450	185.275	89.671	-10.314
2000	14.517	81.067	69.618	22.899	184.794	84.640	-9.249

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 11.605 + 1.828\text{x}10^{-3}T - 1.088\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 11.605\text{x}10^{-3}T + 0.914\text{x}10^{-6}T^{2} + 1.088\text{x}10^{2}T^{-1} - 3.906$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 190.696 - 0.154\text{x}10^{-3}T - 1.310\text{x}10^{-6}T^{2} - 457.300T^{-1}$

$\Delta Gf^\circ = 190.696 + 0.154\text{x}10^{-3}T\ln T + 1.310\text{x}10^{-6}T^{2} - 228.650T^{-1} - 56.773\text{x}10^{-3}T$

Source: Data from Gurvich (196).

$B_2C(g)$
Diboron Carbide (ideal gas)
[Formation: $2B(\beta) + C(c) = B_2C(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.049	53.807	53.807	0	186.300	171.507	-125.717
300	11.060	53.875	53.807	.021	186.307	171.418	-124.876
400	11.672	57.142	54.247	1.158	186.566	166.406	-90.919
500	12.224	59.807	55.101	2.353	186.630	161.360	-70.529
600	12.691	62.078	56.080	3.599	186.549	156.307	-56.934
700	13.072	64.064	57.081	4.888	186.378	151.281	-47.232
800	13.377	65.831	58.067	6.211	186.150	146.284	-39.963
900	13.620	67.421	59.020	7.561	185.875	141.316	-34.316
1000	13.814	68.866	59.932	8.934	185.565	136.384	-29.806
1100	13.971	70.190	60.805	10.323	185.222	131.480	-26.122
1200	14.098	71.411	61.639	11.727	184.850	126.604	-23.058
1300	14.201	72.544	62.435	13.142	184.447	121.773	-20.472
1400	14.287	73.600	63.196	14.566	184.016	116.966	-18.259
1500	14.359	74.588	63.922	15.999	183.555	112.201	-16.348
1600	14.420	75.517	64.618	17.438	183.064	107.437	-14.675
1700	14.472	76.392	65.285	18.882	182.542	102.727	-13.206
1800	14.517	77.221	65.925	20.332	181.993	98.072	-11.907
1900	14.557	78.007	66.541	21.786	181.415	93.428	-10.747
2000	14.593	78.755	67.133	23.243	180.806	88.786	-9.702

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.117 + 1.598\times10^{-3}T - 1.373\times10^{5}T^{-2}$

$H°- H^\circ_{298} = 12.117\times10^{-3}T + 0.799\times10^{-6}T^{2} + 1.373\times10^{2}T^{-1} - 4.144$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 188.276 - 0.847\times10^{-3}T - 1.351\times10^{-6}T^{2} - 478.000T^{-1}$

$\Delta Gf° = 88.276 + 0.847\times10^{-3}T\ln T + 1.351\times10^{-6}T^{2} - 239.000T^{-1} - 58.782\times10^{-3}T$

Source: Data from Gurvich (196).

$B_4C(c,l)$
Tetraboron Carbide
[Formation: $4B(\beta,l) + C(c) = B_4C(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	12.620	6.480	6.480	0	-17.000	-16.841	12.345
300	12.770	6.559	6.482	.023	-17.001	-16.837	12.266
400	18.284	11.069	7.057	1.605	-16.931	-16.797	9.178
500	21.339	15.505	8.309	3.598	-16.883	-16.762	7.327
600	23.325	19.582	9.852	5.838	-16.920	-16.745	6.099
700	24.761	23.291	11.512	8.245	-17.009	-16.705	5.215
800	25.869	26.672	13.198	10.779	-17.118	-16.648	4.548
900	26.758	29.772	14.870	13.412	-17.248	-16.583	4.027
1000	27.494	32.631	16.505	16.126	-17.393	-16.499	3.606
1100	28.117	35.281	18.093	18.907	-17.552	-16.416	3.261
1200	28.655	37.752	19.630	21.746	-17.727	-16.310	2.970
1300	29.130	40.064	21.113	24.636	-17.923	-16.169	2.718
1400	29.560	42.239	22.545	27.571	-18.139	-16.028	2.502
1500	29.959	44.292	23.927	30.547	-18.383	-15.852	2.310
1600	30.343	46.238	25.262	33.562	-18.654	-15.723	2.148
1700	30.724	48.089	26.551	36.615	-18.951	-15.529	1.996
1800	31.114	49.856	27.797	39.707	-19.270	-15.270	1.854
1900	31.524	51.549	29.002	42.839	-19.610	-15.033	1.729
2000	31.967	53.177	30.170	46.013	-19.970	-14.834	1.621
2100	32.453	54.749	31.304	49.234	-20.343	-14.528	1.512
2200	32.993	56.270	32.404	52.505	-20.726	-14.280	1.419
2300	33.598	57.750	33.474	55.834	-21.111	-13.930	1.324
2350	33.938	58.476	33.998	57.523	-21.302	-13.841	1.287
2350	33.938	58.476	33.998	57.523	-69.302	-13.841	1.287
2400	34.278	59.194	34.516	59.228	-69.404	-12.622	1.149
2500	35.045	60.609	35.532	62.693	-69.556	-10.316	.902
2600	35.909	62.000	36.523	66.240	-69.631	-7.884	.663
2700	36.880	63.373	37.492	69.878	-69.618	-5.542	.449
2740	37.300	63.918	37.873	71.362	-69.585	-4.591	.366
2740	32.500	73.042	37.873	96.362	-44.585	-4.591	.366
2800	32.500	73.746	38.635	98.312	-44.812	-3.744	.292
2900	32.500	74.887	39.866	101.562	-45.193	-2.192	.165
3000	32.500	75.988	41.051	104.812	-45.578	-.752	.055

Phase changes: 2350 K, melting point of B; ΔH° = 12.000 kcal/mol.
2740 K, melting point of B_4C; ΔH° = 25.000 kcal/mol.

Heat Capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2740 K: $Cp° = 23.672 + 4.544x10^{-3}T - 11.030x10^{5}T^{-2}$
$H°-H°_{298} = 23.672x10^{-3}T + 2.272x10^{-6}T^{2} + 11.030x10^{2}T^{-1} - 10.959$
2740-3000 K: $Cp° = 32.500$
$H°-H°_{298} = 32.500x10^{-3}T + 7.312$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -17.414 + 1.262x10^{-3}T - 1.262x10^{-6}T^{2} + 44.700T^{-1}$
$\Delta Gf° = -17.414 - 1.262x10^{-3}T\ln T + 1.262x10^{-6}T^{2} + 22.350T^{-1} + 8.483x10^{-3}T$
2000-2350 K: $\Delta Hf° = -15.422 - 0.861x10^{-3}T - 0.630x10^{-6}T^{2} - 503.000T^{-1}$
$\Delta Gf° = -15.422 + 0.861x10^{-3}T\ln T + 0.630x10^{-6}T^{2} - 251.500T^{-1} - 7.317x10^{-3}T$
2350-2740 K: $\Delta Hf° = -52.982 - 11.969x10^{-3}T + 2.138x10^{-6}T^{2} + 383.000T^{-1}$
$\Delta Gf° = -52.982 + 11.969x10^{-3}T\ln T - 2.138x10^{-6}T^{2} + 191.500T^{-1} - 71.132x10^{-3}T$
2740-3000 K: $\Delta Hf° = -34.711 - 3.141x10^{-3}T - 0.134x10^{-6}T^{2} - 720.000T^{-1}$
$\Delta Gf° = -34.711 + 3.141x10^{-3}T\ln T + 0.134x10^{-6}T^{2} - 360.000T^{-1} - 14.072x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from Kelley (239). High-temperature data based on King (256) and Sheindlin (445).

BH(g)
Boron Hydride (ideal gas)
[Formation: $B(\beta) + 0.5H_2(g) = BH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	6.974	41.043	41.043	0	106.650	99.486	-72.924
300	6.975	41.086	41.043	.013	106.652	99.442	-72.443
400	7.014	43.097	41.317	.712	106.687	97.029	-53.014
500	7.109	44.671	41.835	1.418	106.636	94.622	-41.359
600	7.252	45.979	42.421	2.135	106.528	92.225	-33.593
700	7.423	47.110	43.011	2.869	106.393	89.853	-28.053
800	7.601	48.113	43.588	3.620	106.245	87.501	-23.904
900	7.773	49.018	44.141	4.389	106.090	85.168	-20.681
1000	7.933	49.846	44.672	5.174	105.928	82.852	-18.107
1100	8.080	50.609	45.177	5.975	105.761	80.546	-16.003
1200	8.214	51.318	45.660	6.790	105.590	78.264	-14.254
1300	8.338	51.980	46.120	7.618	105.411	75.998	-12.776
1400	8.458	52.602	46.561	8.457	105.224	73.742	-11.511
1500	8.576	53.190	46.984	9.309	105.029	71.503	-10.418
1600	8.697	53.747	47.389	10.173	104.827	69.263	-9.461
1700	8.824	54.278	47.779	11.049	104.617	67.049	-8.620
1800	8.959	54.786	48.154	11.938	104.402	64.856	-7.875
1900	9.104	55.275	48.517	12.841	104.182	62.666	-7.208
2000	9.261	55.745	48.865	13.759	103.958	60.475	-6.608

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.341 + 1.504\times10^{-3}T + 0.164\times10^{5}T^{-2}$

$H°-H°_{298} = 6.341\times10^{-3}T + 0.752\times10^{-6}T^{2} - 0.164\times10^{2}T^{-1} - 1.902$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 107.914 - 1.610\times10^{-3}T - 0.149\times10^{-6}T^{2} - 229.650T^{-1}$

$\Delta Gf° = 107.914 + 1.610\times10^{-3}T\ln T + 0.149\times10^{-6}T^{2} - 114.825T^{-1} - 36.193\times10^{-3}T$

Source: Data from Gurvich (196).

$BH_2(g)$
Boron Dihydride (ideal gas)
[Formation: $B(\beta) + H_2(g) = BH_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.295	46.217	46.217	0	70.580	66.525	-48.764
300	8.302	46.267	46.217	.015	70.577	66.501	-48.445
400	8.675	48.706	46.546	.864	70.415	65.163	-35.603
500	9.047	50.683	47.183	1.750	70.195	63.877	-27.920
600	9.422	52.365	47.908	2.674	69.944	62.634	-22.814
700	9.806	53.847	48.654	3.635	69.685	61.437	-19.181
800	10.192	55.182	49.388	4.635	69.433	60.277	-16.467
900	10.571	56.404	50.101	5.673	69.191	59.147	-14.363
1000	10.937	57.537	50.788	6.749	68.961	58.044	-12.685
1100	11.282	58.596	51.451	7.860	68.742	56.957	-11.316
1200	11.606	59.592	52.088	9.005	68.532	55.897	-10.180
1300	11.907	60.532	52.700	10.181	68.328	54.857	-9.222
1400	12.185	61.426	53.294	11.385	68.128	53.826	-8.402
1500	12.440	62.275	53.864	12.617	67.930	52.816	-7.695
1600	12.672	63.086	54.415	13.874	67.732	51.802	-7.076
1700	12.883	63.860	54.948	15.150	67.529	50.815	-6.533
1800	13.074	64.602	55.464	16.448	67.324	49.848	-6.052
1900	13.245	65.314	55.964	17.765	67.115	48.885	-5.623
2000	13.399	65.997	56.449	19.097	66.898	47.918	-5.236

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.579 + 3.256\times10^{-3}T - 0.226\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.579\times10^{-3}T + 1.628\times10^{-6}T^{2} + 0.226\times10^{2}T^{-1} - 2.480$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 72.219 - 3.600\times10^{-3}T + 0.517\times10^{-6}T^{2} - 182.400T^{-1}$

$\Delta Gf^\circ = 72.219 + 3.600\times10^{-3}T\ln T - 0.517\times10^{-6}T^{2} - 91.200T^{-1} - 38.429\times10^{-3}T$

Source: Data from Gurvich (196).

$BH_3(g)$
Boron Trihydride (ideal gas)
[Formation: $B(\beta) + 1.5H_2(g) = BH_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.312	44.831	44.831	0	22.000	23.011	-16.867
300	8.321	44.883	44.831	.016	21.992	23.018	-16.768
400	8.982	47.361	45.164	.879	21.497	23.432	-12.803
500	9.826	49.455	45.819	1.818	20.980	23.977	-10.480
600	10.737	51.326	46.583	2.846	20.483	24.621	-8.968
700	11.645	53.049	47.383	3.966	20.032	25.350	-7.914
800	12.506	54.662	48.194	5.174	19.635	26.138	-7.140
900	13.298	56.181	48.999	6.464	19.290	26.971	-6.549
1000	14.009	57.619	49.788	7.831	18.992	27.843	-6.085
1100	14.640	58.986	50.563	9.265	18.733	28.734	-5.709
1200	15.194	60.284	51.321	10.756	18.501	29.655	-5.401
1300	15.679	61.520	52.058	12.301	18.292	30.597	-5.144
1400	16.103	62.697	52.776	13.890	18.099	31.551	-4.925
1500	16.472	63.821	53.474	15.520	17.916	32.522	-4.738
1600	16.795	64.895	54.155	17.184	17.737	33.489	-4.574
1700	17.078	65.922	54.817	18.878	17.558	34.482	-4.433
1800	17.326	66.905	55.462	20.597	17.375	35.492	-4.309
1900	17.545	67.848	56.090	22.341	17.191	36.505	-4.199
2000	17.739	68.753	56.699	24.107	17.000	37.515	-4.099

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.537 + 6.052\times10^{-3}T - 0.915\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.537\times10^{-3}T + 3.026\times10^{-6}T^{2} + 0.915\times10^{2}T^{-1} - 2.823$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 24.250 - 6.870\times10^{-3}T + 1.706\times10^{-6}T^{2} - 105.250T^{-1}$

$\Delta Gf^\circ = 24.250 + 6.870\times10^{-3}T\ln T - 1.706\times10^{-6}T^{2} - 52.625T^{-1} - 42.198\times10^{-3}T$

Source: Data from Gurvich (196).

$B_2H_6(g)$
Diborane (ideal gas)
[Formation: $2B(\beta) + 3H_2(g) = B_2H_6(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	13.886	55.709	55.709	0	9.800	21.944	-16.085
300	13.957	55.795	55.709	.026	9.777	22.022	-16.042
400	17.747	60.335	56.302	1.613	8.648	26.274	-14.355
500	21.196	64.673	57.547	3.563	7.687	30.800	-13.462
600	24.219	68.811	59.081	5.838	6.912	35.493	-12.928
700	26.835	72.746	60.755	8.394	6.326	40.308	-12.585
800	29.077	76.480	62.490	11.192	5.914	45.195	-12.346
900	30.984	80.018	64.242	14.198	5.649	50.122	-12.171
1000	32.600	83.368	65.989	17.379	5.500	55.072	-12.036
1100	33.966	86.541	67.715	20.709	5.444	60.020	-11.925
1200	35.123	89.547	69.410	24.165	5.454	64.988	-11.836
1300	36.105	92.399	71.070	27.728	5.511	69.953	-11.760
1400	36.941	95.106	72.690	31.382	5.601	74.907	-11.693
1500	37.656	97.679	74.271	35.112	5.704	79.861	-11.636
1600	38.271	100.130	75.812	38.909	5.814	84.774	-11.579
1700	38.802	102.466	77.311	42.764	5.924	89.714	-11.533
1800	39.262	104.697	78.771	46.667	6.024	94.660	-11.493
1900	39.664	106.831	80.192	50.614	6.113	99.585	-11.455
2000	40.016	108.875	81.576	54.599	6.185	104.477	-11.417

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.605 + 12.248\times10^{-3}T - 8.330\times10^{5}T^{-2}$

$H°-H°_{298} = 19.605\times10^{-3}T + 6.124\times10^{-6}T^{2} + 8.330\times10^{2}T^{-1} - 9.184$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 10.762 - 9.209\times10^{-3}T + 3.483\times10^{-6}T^{2} + 439.500T^{-1}$

$\Delta Gf° = 10.762 + 9.209\times10^{-3}T\ln T - 3.483\times10^{-6}T^{2} + 219.750T^{-1} - 16.397\times10^{-3}T$

Source: Data from JANAF (127).

$B_5H_9(l,g)$
Pentaborane
[Formation: $5B(\beta) + 4.5H_2(g) = B_5H_9(l,g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	36.120	44.056	44.056	0	10.240	41.076	-30.109
300	36.400	44.280	44.057	.067	10.224	41.272	-30.066
335	39.200	48.331	44.286	1.355	9.927	44.914	-29.301
335	25.574	68.600	44.287	8.145	16.717	44.914	-29.301
400	31.120	73.631	48.643	9.995	15.444	50.496	-27.589
500	38.568	81.397	54.419	13.489	13.757	59.472	-25.995
600	44.841	89.000	59.552	17.669	12.412	68.733	-25.036
700	50.047	96.316	64.286	22.421	11.415	78.210	-24.418
800	54.342	103.289	68.729	27.648	10.735	87.809	-23.988
900	57.882	109.901	72.940	33.265	10.308	97.470	-23.669
1000	60.805	116.155	76.951	39.204	10.076	107.171	-23.422
1100	63.227	122.068	80.787	45.409	9.994	116.854	-23.216
1200	65.245	127.658	84.461	51.836	10.014	126.582	-23.053
1300	66.936	132.949	87.990	58.447	10.097	136.309	-22.915
1400	68.361	137.964	91.383	65.214	10.222	146.010	-22.793
1500	69.569	142.722	94.647	72.112	10.354	155.724	-22.689
1600	70.600	147.246	97.795	79.122	10.477	165.348	-22.585
1700	71.486	151.553	100.831	86.227	10.581	175.036	-22.502
1800	72.250	155.661	103.764	93.415	10.652	184.762	-22.433
1900	72.914	159.586	106.600	100.674	10.685	194.442	-22.366
2000	73.494	163.341	109.344	107.995	10.668	204.049	-22.297

Phase change: 335 K, boiling point of B_5H_9; ΔH° = 6.790 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-335 K: $Cp° = 25.590 + 35.316 \times 10^{-3}T$
$H° - H°_{298} = 25.590 \times 10^{-3}T + 17.658 \times 10^{-6}T^2 - 9.199$
335-2000 K: $Cp° = 40.733 + 19.900 \times 10^{-3}T - 24.494 \times 10^{5}T^{-2}$
$H° - H°_{298} = 40.733 \times 10^{-3}T + 9.950 \times 10^{-6}T^2 + 24.494 \times 10^{2}T^{-1} - 13.929$

Formation equations (kcal/mol):

298.15-335 K: $\Delta Hf° = 20.684 - 27.077 \times 10^{-3}T + 12.313 \times 10^{-6}T^2 - 1033.250T^{-1}$
$\Delta Gf° = 20.684 + 27.077 \times 10^{-3}T\ln T - 12.313 \times 10^{-6}T^2 - 516.625T^{-1} - 76.395 \times 10^{-3}T$
335-2000 K: $\Delta Hf° = 15.955 - 11.934 \times 10^{-3}T + 4.605 \times 10^{-6}T^2 + 1416.150T^{-1}$
$\Delta Gf° = 15.955 + 11.934 \times 10^{-3}T\ln T - 4.605 \times 10^{-6}T^2 + 708.075T^{-1} + 12.271 \times 10^{-3}T$

Source: Data from JANAF (127).

$B_{10}H_{14}$(c,l,g)
Decaborane (ideal gas)
[Formation: $10B(\beta) + 7H_2(g) = B_{10}H_{14}(c,l,g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	52.092	42.200	42.200	0	-10.800	45.953	-33.684
300	52.511	42.524	42.201	.097	-10.844	46.314	-33.739
371.93	67.200	55.896	43.663	4.550	-12.063	60.101	-35.316
371.93	70.500	70.012	43.663	9.800	-6.813	60.101	-35.316
400	77.200	75.385	45.680	11.882	-7.087	65.171	-35.607
492	82.500	91.909	52.803	19.240	-7.948	81.907	-36.383
492	72.158	112.844	52.803	29.540	2.352	81.907	-36.383
500	73.238	114.017	53.765	30.126	2.194	83.206	-36.369
600	84.050	128.362	65.010	38.011	.429	99.556	-36.263
700	92.719	141.994	75.044	46.865	-.811	116.197	-36.278
800	99.711	154.848	84.224	56.499	-1.579	132.982	-36.328
900	105.389	166.931	92.749	66.764	-1.981	149.828	-36.383
1000	110.031	178.284	100.742	77.542	-2.109	166.707	-36.433
1100	113.852	188.956	108.281	88.742	-2.031	183.526	-36.463
1200	117.019	199.002	115.426	100.291	-1.824	200.411	-36.499
1300	119.663	208.476	122.223	112.129	-1.548	217.286	-36.529
1400	121.885	217.428	128.707	124.209	-1.240	234.103	-36.545
1500	123.766	225.903	134.907	136.494	-.954	250.941	-36.562
1600	125.369	233.943	140.847	148.953	-.714	267.601	-36.552
1700	126.743	241.586	146.550	161.561	-.535	284.385	-36.560
1800	127.929	248.865	152.034	174.296	-.439	301.252	-36.576
1900	128.957	255.809	157.314	187.141	-.436	318.031	-36.581
2000	129.854	262.447	162.406	200.083	-.539	334.665	-36.570

Phase changes: 371.93 K, melting point of $B_{10}H_{14}$; ΔH° = 5.250 kcal/mol.
492 K, boiling point of $B_{10}H_{14}$; ΔH° = 10.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-371.93 K: $Cp° = -25.316 + 259.632\times10^{-3}T$
$H°-H°_{298} = -25.316\times10^{-3}T + 129.816\times10^{-6}T^2 - 3.992$

371.93-492 K: $Cp° = 36.841 + 96.720\times10^{-3}T$
$H°-H°_{298} = 36.841\times10^{-3}T + 48.360\times10^{-6}T^2 - 10.592$

492-2000 K: $Cp° = 98.637 + 18.858\times10^{-3}T - 86.556\times10^{5}T^{-2}$
$H°-H°_{298} = 98.637\times10^{-3}T + 9.429\times10^{-6}T^2 + 86.556\times10^{2}T^{-1} - 38.865$

Formation equations (kcal/mol):

298.15-371.93 K: $\Delta Hf° = 20.681 - 117.738\times10^{-3}T + 119.963\times10^{-6}T^2 - 2099.500T^{-1}$
$\Delta Gf° = 20.681 + 117.738\times10^{-3}T\ln T - 119.963\times10^{-6}T^2 - 1049.750T^{-1} - 538.488\times10^{-3}T$

371.93-492 K: $\Delta Hf° = 14.081 - 55.581\times10^{-3}T + 38.507\times10^{-6}T^2 - 2099.500T^{-1}$
$\Delta Gf° = 14.081 + 55.581\times10^{-3}T\ln T - 38.507\times10^{-6}T^2 - 1049.750T^{-1} - 183.149\times10^{-3}T$

492-2000 K: $\Delta Hf° = -14.191 + 6.215\times10^{-3}T - 0.424\times10^{-6}T^2 + 6556.100T^{-1}$
$\Delta Gf° = -14.191 - 6.215\times10^{-3}T\ln T + 0.424\times10^{-6}T^2 + 3278.050T^{-1} + 220.324\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data from JANAF (127).

$BH_3NH_3(g)$
Borane Monoammoniate (ideal gas)
[Formation: $B(\beta) + 3H_2(g) + 0.5N_2(g) = BH_3NH_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	13.615	57.543	57.543	0	-27.500	-9.500	6.963
300	13.667	57.628	57.545	.025	-27.526	-9.388	6.839
400	16.630	61.966	58.116	1.540	-28.758	-3.152	1.722
500	19.538	65.992	59.294	3.349	-29.805	3.375	-1.475
600	22.181	69.792	60.732	5.436	-30.649	10.089	-3.675
700	24.524	73.391	62.287	7.773	-31.300	16.933	-5.287
800	26.580	76.800	63.890	10.328	-31.780	23.860	-6.518
900	28.375	80.039	65.506	13.080	-32.110	30.836	-7.488
1000	29.939	83.115	67.111	16.004	-32.315	37.844	-8.271
1100	31.300	86.039	68.695	19.078	-32.417	44.865	-8.914
1200	32.485	88.820	70.252	22.282	-32.440	51.904	-9.453
1300	33.534	91.453	71.787	25.566	-32.434	58.930	-9.907
1400	34.437	93.974	73.280	28.972	-32.354	65.958	-10.296
1500	35.226	96.380	74.737	32.464	-32.240	72.984	-10.634
1600	35.917	98.679	76.159	36.032	-32.099	79.985	-10.925
1700	36.537	100.869	77.554	39.636	-31.970	86.983	-11.182
1800	37.072	102.974	78.907	43.321	-31.806	93.987	-11.411
1900	37.545	104.992	80.226	47.056	-31.635	100.976	-11.615
2000	37.964	106.930	81.511	50.837	-31.463	107.940	-11.795

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.363 + 14.832\times10^{-3}T - 4.596\times10^{5}T^{-2}$

$H°- H°_{298} = 14.363\times10^{-3}T + 7.416\times10^{-6}T^{2} + 4.596\times10^{2}T^{-1} - 6.483$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -25.066 - 12.986\times10^{-3}T + 5.173\times10^{-6}T^{2} + 291.550T^{-1}$

$\Delta Gf° = -25.066 + 12.986\times10^{-3}T\ln T - 5.173\times10^{-6}T^{2} + 145.775T^{-1} - 21.881\times10^{-3}T$

Source: Data from Gurvich (196).

BN(hexagonal)
Boron Nitride
[Formation: $B(\beta) + 0.5N_2(g) = BN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	4.715	3.607	3.607	0	-60.800	-54.632	40.046
300	4.751	3.636	3.607	.009	-60.803	-54.592	39.770
400	6.314	5.231	3.813	.567	-60.910	-52.507	28.688
500	7.460	6.769	4.253	1.258	-60.978	-50.396	22.028
600	8.369	8.212	4.794	2.051	-61.016	-48.278	17.585
700	9.110	9.560	5.380	2.926	-61.022	-46.152	14.409
800	9.717	10.817	5.981	3.869	-60.997	-44.027	12.028
900	10.211	11.991	6.584	4.866	-60.948	-41.909	10.177
1000	10.608	13.089	7.181	5.908	-60.882	-39.797	8.698
1100	10.919	14.115	7.765	6.985	-60.803	-37.698	7.490
1200	11.157	15.076	8.335	8.089	-60.718	-35.600	6.484
1300	11.333	15.976	8.888	9.214	-60.632	-33.506	5.633
1400	11.455	16.821	9.425	10.354	-60.551	-31.423	4.905
1500	11.535	17.614	9.945	11.504	-60.479	-29.341	4.275
1600	11.582	18.360	10.448	12.660	-60.418	-27.279	3.726
1700	11.605	19.063	10.934	13.819	-60.373	-25.209	3.241
1800	11.613	19.726	11.404	14.980	-60.342	-23.129	2.808
1900	11.617	20.354	11.858	16.142	-60.326	-21.060	2.422
2000	11.626	20.950	12.298	17.304	-60.327	-19.007	2.077
2100	11.648	21.518	12.724	18.467	-60.344	-16.931	1.762
2200	11.694	22.061	13.136	19.634	-60.371	-14.873	1.477

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2200 K: $C_p^\circ = 8.183 + 2.264\times10^{-3}T - 3.683\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 8.183\times10^{-3}T + 1.132\times10^{-6}T^2 + 3.683\times10^{2}T^{-1} - 3.776$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -61.379 + 0.202\times10^{-3}T + 0.145\times10^{-6}T^2 + 150.750T^{-1}$
$\Delta Gf^\circ = -61.379 - 0.202\times10^{-3}T\ln T - 0.145\times10^{-6}T^2 + 75.375T^{-1} + 22.972\times10^{-3}T$
2000-2200 K: $\Delta Hf^\circ = -60.042 - 0.863\times10^{-3}T + 0.412\times10^{-6}T^2 - 399.200T^{-1}$
$\Delta Gf^\circ = -60.042 + 0.863\times10^{-3}T\ln T - 0.412\times10^{-6}T^2 - 199.600T^{-1} + 14.818\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from Sirota (462). High-temperature data based on McDonald (326) and Prophet (409).

BN(g)
Boron Nitride (ideal gas)
[Formation: $B(\beta) + 0.5N_2(g) = BN(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.063	50.689	50.689	0	118.100	110.231	-80.800
300	7.065	50.732	50.689	.013	118.102	110.183	-80.267
400	7.247	52.787	50.967	.728	118.151	107.532	-58.752
500	7.492	54.430	51.502	1.464	118.128	104.880	-45.842
600	7.738	55.818	52.108	2.226	118.059	102.234	-37.238
700	7.961	57.028	52.727	3.011	117.963	99.605	-31.098
800	8.160	58.104	53.333	3.817	117.851	96.991	-26.496
900	8.342	59.076	53.917	4.643	117.728	94.391	-22.921
1000	8.513	59.964	54.478	5.486	117.596	91.806	-20.064
1100	8.678	60.783	55.015	6.345	117.457	89.227	-17.728
1200	8.837	61.545	55.528	7.221	117.314	86.669	-15.784
1300	8.992	62.258	56.018	8.112	117.165	84.125	-14.143
1400	9.141	62.930	56.488	9.019	117.014	81.589	-12.736
1500	9.283	63.565	56.938	9.940	116.857	79.069	-11.520
1600	9.418	64.169	57.372	10.875	116.697	76.541	-10.455
1700	9.544	64.744	57.789	11.824	116.532	74.038	-9.518
1800	9.660	65.293	58.191	12.784	116.362	71.555	-8.688
1900	9.766	65.818	58.579	13.755	116.186	69.071	-7.945
2000	9.861	66.321	58.952	14.737	116.006	66.585	-7.276

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.770 + 1.694x10^{-3}T - 0.188x10^{5}T^{-2}$

$H°- H°_{298} = 6.770x10^{-3}T + 0.847x10^{-6}T^{2} + 0.188x10^{2}T^{-1} - 2.157$

Formation equations (kcal/mol):

298.15-2000 K: $ΔHf° = 119.140 - 1.211x10^{-3}T - 0.140x10^{-6}T^{2} - 198.750T^{-1}$

$ΔGf° = 119.140 + 1.211x10^{-3}TlnT + 0.140x10^{-6}T^{2} - 99.375T^{-1} - 35.709x10^{-3}T$

Source: Data from Gurvich (196).

BOBr(g)
Boron Oxybromide (ideal gas)
[Formation: $B(\beta) + 0.5O_2(g) + 0.5Br_2(l,g) = BOBr(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	11.188	59.463	59.463	0	-60.000	-64.580	47.338
300	11.206	59.532	59.463	.021	-60.007	-64.607	47.065
332.6	11.455	60.701	59.527	.390	-60.139	-65.100	42.776
332.6	11.455	60.701	59.527	.390	-63.671	-65.100	42.776
400	11.969	62.869	59.914	1.182	-63.639	-65.397	35.731
500	12.498	65.600	60.786	2.407	-63.627	-65.836	28.777
600	12.909	67.916	61.786	3.678	-63.653	-66.278	24.142
700	13.239	69.932	62.809	4.986	-63.699	-66.711	20.828
800	13.505	71.718	63.813	6.324	-63.753	-67.137	18.341
900	13.720	73.321	64.781	7.686	-63.817	-67.556	16.405
1000	13.893	74.776	65.710	9.066	-63.888	-67.968	14.854
1100	14.034	76.107	66.595	10.463	-63.965	-68.378	13.585
1200	14.149	77.333	67.440	11.872	-64.051	-68.773	12.525
1300	14.244	78.470	68.245	13.292	-64.146	-69.160	11.627
1400	14.323	79.528	69.013	14.721	-64.250	-69.541	10.856
1500	14.390	80.519	69.748	16.156	-64.367	-69.913	10.186
1600	14.445	81.449	70.450	17.598	-64.495	-70.289	9.601
1700	14.493	82.326	71.123	19.045	-64.637	-70.646	9.082
1800	14.534	83.156	71.769	20.497	-64.790	-70.983	8.618
1900	14.569	83.943	72.389	21.952	-64.958	-71.321	8.204
2000	14.599	84.691	72.986	23.410	-65.141	-71.665	7.831

*Data estimated.

Phase change: 332.60 K, Boiling point of Br_2 ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 12.686 + 1.210\times10^{-3}T - 1.652\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.686\times10^{-3}T + 0.605\times10^{-6}T^2 + 1.652\times10^{2}T^{-1} - 4.390$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -58.309 - 4.697\times10^{-3}T - 0.288\times10^{-6}T^2 - 78.900T^{-1}$

$\Delta Gf^\circ = -58.309 + 4.697\times10^{-3}T\ln T + 0.288\times10^{-6}T^2 - 39.450T^{-1} - 47.439\times10^{-3}T$

332.60-2000 K: $\Delta Hf^\circ = -63.309 - 0.117\times10^{-3}T - 0.366\times10^{-6}T^2 - 94.600T^{-1}$

$\Delta Gf^\circ = -63.309 + 0.117\times10^{-3}T\ln T + 0.366\times10^{-6}T^2 - 47.300T^{-1} - 5.761\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

BOCl(g)
Boron Oxychloride (ideal gas)
[Formation: $B(\beta) + 0.5O_2(g) + 0.5Cl_2(g) = BOCl(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	10.765	56.720	56.720	0	-75.600	-76.841	56.325
300	10.785	56.786	56.720	.020	-75.599	-76.847	55.983
400	11.642	60.015	57.155	1.144	-75.562	-77.273	42.219
500	12.241	62.681	58.001	2.340	-75.565	-77.698	33.961
600	12.703	64.955	58.975	3.588	-75.604	-78.124	28.456
700	13.069	66.942	59.975	4.877	-75.661	-78.539	24.521
800	13.363	68.707	60.958	6.199	-75.727	-78.945	21.567
900	13.599	70.295	61.908	7.548	-75.799	-79.342	19.267
1000	13.790	71.738	62.820	8.918	-75.878	-79.731	17.425
1100	13.945	73.060	63.692	10.305	-75.963	-80.119	15.918
1200	14.072	74.279	64.524	11.706	-76.054	-80.491	14.659
1300	14.176	75.409	65.318	13.118	-76.156	-80.853	13.592
1400	14.263	76.463	66.077	14.541	-76.264	-81.210	12.677
1500	14.336	77.450	66.803	15.971	-76.385	-81.556	11.883
1600	14.398	78.377	67.498	17.407	-76.520	-81.909	11.188
1700	14.450	79.251	68.163	18.850	-76.665	-82.238	10.572
1800	14.495	80.079	68.803	20.297	-76.823	-82.551	10.023
1900	14.534	80.864	69.417	21.749	-76.994	-82.863	9.531
2000	14.568	81.610	70.008	23.204	-77.180	-83.180	9.089

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.359 + 1.420x10^{-3}T - 1.793x10^{5}T^{-2}$
$H°-H°_{298} = 12.359x10^{-3}T + 0.710x10^{-6}T^{2} + 1.793x10^{2}T^{-1} - 4.349$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -75.126 - 0.393x10^{-3}T - 0.278x10^{-6}T^{2} - 98.950T^{-1}$
$\Delta Gf° = -75.126 + 0.393x10^{-3}T\ln T + 0.278x10^{-6}T^{2} - 49.475T^{-1} - 7.513x10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$(BOCl)_3(g)$
Trimeric Boron Oxychloride (ideal gas)
[Formation: $3B(\beta) + 1.5O_2(g) + 1.5Cl_2(g) = (BOCl)_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	31.436	91.367	91.367	0	-390.000	-370.231	271.383
300	31.538	91.562	91.369	.058	-389.999	-370.106	269.618
400	36.260	101.318	92.666	3.461	-389.857	-363.499	198.604
500	39.618	109.792	95.262	7.265	-389.650	-356.923	156.009
600	41.975	117.236	98.318	11.351	-389.425	-350.408	127.634
700	43.646	123.839	101.500	15.637	-389.177	-343.919	107.375
800	44.854	129.750	104.669	20.065	-388.913	-337.471	92.192
900	45.747	135.087	107.757	24.597	-388.644	-331.056	80.390
1000	46.421	139.943	110.736	29.207	-388.379	-324.670	70.956
1100	46.940	144.393	113.597	33.876	-388.126	-318.330	63.245
1200	47.347	148.496	116.337	38.591	-387.891	-311.990	56.820
1300	47.672	152.299	118.958	43.343	-387.678	-305.664	51.386
1400	47.934	155.842	121.468	48.124	-387.493	-299.363	46.732
1500	48.149	159.156	123.871	52.928	-387.341	-293.062	42.699
1600	48.327	162.270	126.175	57.752	-387.229	-286.818	39.177
1700	48.476	165.204	128.385	62.593	-387.151	-280.538	36.065
1800	48.602	167.978	130.507	67.447	-387.113	-274.232	33.296
1900	48.709	170.609	132.550	72.312	-387.117	-267.957	30.822
2000	48.802	173.110	134.516	77.188	-387.164	-261.724	28.600

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 42.654 + 4.114\times10^{-3}T - 11.063\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 42.654\times10^{-3}T + 2.057\times10^{-6}T^{2} + 11.063\times10^{2}T^{-1} - 16.611$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -392.142 + 4.399\times10^{-3}T - 0.905\times10^{-6}T^{2} + 271.550T^{-1}$

$\Delta Gf^\circ = -392.142 - 4.399\times10^{-3}T\ln T + 0.905\times10^{-6}T^{2} + 135.775T^{-1} + 96.759\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$BOF(g)$
Boron Oxyfluoride (ideal gas)
[Formation: $B(\beta) + 0.5O_2(g) + 0.5F_2(g) = BOF(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	9.798	53.705	53.705	0	-144.000	-145.065	106.334
300	9.819	53.766	53.706	.018	-144.000	-145.071	105.682
400	10.792	56.730	54.103	1.051	-144.024	-145.426	79.456
500	11.540	59.222	54.884	2.169	-144.080	-145.768	63.714
600	12.130	61.380	55.790	3.354	-144.163	-146.100	53.216
700	12.600	63.287	56.728	4.591	-144.257	-146.415	45.712
800	12.975	64.995	57.656	5.871	-144.353	-146.716	40.080
900	13.275	66.541	58.559	7.184	-144.451	-147.005	35.697
1000	13.515	67.952	59.428	8.524	-144.553	-147.282	32.188
1100	13.710	69.250	60.264	9.885	-144.659	-147.557	29.316
1200	13.869	70.450	61.063	11.264	-144.768	-147.814	26.920
1300	14.000	71.565	61.828	12.658	-144.883	-148.059	24.891
1400	14.109	72.607	62.561	14.064	-145.008	-148.300	23.150
1500	14.200	73.584	63.265	15.479	-145.142	-148.527	21.640
1600	14.277	74.503	63.939	16.903	-145.288	-148.760	20.319
1700	14.342	75.370	64.585	18.334	-145.443	-148.970	19.151
1800	14.398	76.192	65.208	19.771	-145.613	-149.162	18.111
1900	14.446	76.971	65.806	21.214	-145.793	-149.351	17.179
2000	14.487	77.713	66.383	22.660	-145.989	-149.547	16.342

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.605 + 1.860\times10^{-3}T - 2.099\times10^{5}T^{-2}$

$H°-H°_{298} = 11.605\times10^{-3}T + 0.930\times10^{-6}T^{2} + 2.099\times10^{2}T^{-1} - 4.247$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -143.414 - 0.987\times10^{-3}T - 0.101\times10^{-6}T^{2} - 84.450T^{-1}$

$\Delta Gf° = -143.414 + 0.987\times10^{-3}T\ln T + 0.101\times10^{-6}T^{2} - 42.225T^{-1} - 10.716\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$(BOF)_3(g)$
Trimeric Boron Oxyfluoride (ideal gas)
[Formation: $3B(\beta) + 1.5O_2(g) + 1.5F_2(g) = (BOF)_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	27.489	81.825	81.825	0	-565.300	-544.854	399.383
300	27.590	81.995	81.825	.051	-565.304	-544.724	396.826
400	32.456	90.626	82.968	3.063	-565.462	-537.842	293.860
500	36.226	98.292	85.282	6.505	-565.543	-530.919	232.062
600	39.066	105.161	88.033	10.277	-565.574	-523.999	190.864
700	41.189	111.350	90.929	14.295	-565.549	-517.066	161.433
800	42.783	116.959	93.838	18.497	-565.475	-510.144	139.363
900	43.994	122.071	96.694	22.839	-565.367	-503.231	122.200
1000	44.927	126.757	99.470	27.287	-565.244	-496.334	108.472
1100	45.657	131.074	102.149	31.817	-565.113	-489.465	97.247
1200	46.237	135.073	104.729	36.413	-564.983	-482.589	87.890
1300	46.703	138.793	107.208	41.061	-564.864	-475.717	79.974
1400	47.083	142.268	109.589	45.751	-564.763	-468.866	73.192
1500	47.396	145.528	111.878	50.475	-564.688	-462.008	67.314
1600	47.657	148.595	114.077	55.228	-564.643	-455.199	62.177
1700	47.876	151.491	116.194	60.005	-564.628	-448.355	57.639
1800	48.062	154.233	118.232	64.802	-564.648	-441.480	53.602
1900	48.221	156.836	120.195	69.617	-564.704	-434.631	49.993
2000	48.358	159.313	122.090	74.446	-564.801	-427.823	46.750

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 37.930 + 6.950 \times 10^{-3}T - 11.123 \times 10^{5}T^{-2}$

$H° - H°_{298} = 37.930 \times 10^{-3}T + 3.475 \times 10^{-6}T^{2} + 11.123 \times 10^{2}T^{-1} - 15.348$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -566.149 + 0.154 \times 10^{-3}T + 0.384 \times 10^{-6}T^{2} + 229.250T^{-1}$

$\Delta Gf° = -566.149 - 0.154 \times 10^{-3}T\ln T - 0.384 \times 10^{-6}T^{2} + 114.625T^{-1} + 71.127 \times 10^{-3}T$

Source: Data from JANAF (127) who estimated most molecular constants.

$BOF_2(g)$
Boron Oxide Difluoride (ideal gas)
[Formation: $B(\beta) + 0.5O_2(g) + F_2(g) = BOF_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	11.998	63.989	63.989	0	-200.000	-196.909	144.336
300	12.036	64.063	63.990	.022	-200.003	-196.889	143.432
400	13.900	67.792	64.484	1.323	-200.144	-195.830	106.995
500	15.307	71.053	65.479	2.787	-200.256	-194.736	85.118
600	16.330	73.939	66.654	4.371	-200.354	-193.626	70.527
700	17.072	76.515	67.881	6.044	-200.436	-192.495	60.099
800	17.618	78.832	69.108	7.779	-200.508	-191.356	52.275
900	18.026	80.932	70.306	9.563	-200.572	-190.207	46.188
1000	18.337	82.848	71.467	11.381	-200.635	-189.053	41.317
1100	18.577	84.608	72.583	13.228	-200.698	-187.897	37.331
1200	18.767	86.232	73.653	15.095	-200.764	-186.728	34.007
1300	18.919	87.741	74.679	16.980	-200.837	-185.552	31.194
1400	19.042	89.148	75.664	18.878	-200.919	-184.375	28.782
1500	19.143	90.465	76.607	20.787	-201.010	-183.187	26.690
1600	19.227	91.703	77.512	22.706	-201.114	-182.006	24.861
1700	19.298	92.871	78.382	24.632	-201.229	-180.807	23.244
1800	19.358	93.976	79.218	26.565	-201.358	-179.591	21.805
1900	19.409	95.024	80.022	28.504	-201.499	-178.375	20.518
2000	19.453	96.020	80.796	30.447	-201.656	-177.166	19.360

*Enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 16.390 + 2.026\times10^{-3}T - 4.442\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.390\times10^{-3}T + 1.013\times10^{-6}T^{2} + 4.442\times10^{2}T^{-1} - 6.467$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -200.189 - 0.456\times10^{-3}T - 0.105\times10^{-6}T^{2} + 99.600T^{-1}$

$\Delta Gf^\circ = -200.189 + 0.456\times10^{-3}T\ln T + 0.105\times10^{-6}T^{2} + 49.800T^{-1} + 7.810\times10^{-3}T$

Source: Data from JANAF (127) who estimated enthalpy of formation at 298 K.

$B_3O_3H_3(g)$
Boroxin (ideal gas)
[Formation: $3B(\beta) + 1.5O_2(g) + 1.5H_2(g) = B_3O_3H_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	20.992	69.744	69.744	0	-291.000	-274.660	201.329
300	21.084	69.874	69.744	.039	-291.015	-274.556	200.011
400	25.753	76.594	70.629	2.386	-291.725	-268.964	146.953
500	29.706	82.779	72.449	5.165	-292.312	-263.196	115.042
600	32.920	88.490	74.653	8.302	-292.783	-257.335	93.733
700	35.514	93.767	77.011	11.729	-293.129	-251.393	78.488
800	37.614	98.651	79.415	15.389	-293.363	-245.412	67.043
900	39.326	103.183	81.806	19.239	-293.508	-239.408	58.135
1000	40.731	107.402	84.158	23.244	-293.585	-233.392	51.007
1100	41.891	111.340	86.452	27.377	-293.611	-227.388	45.177
1200	42.856	115.028	88.682	31.615	-293.606	-221.362	40.315
1300	43.664	118.491	90.843	35.943	-293.583	-215.331	36.200
1400	44.345	121.752	92.935	40.344	-293.556	-209.314	32.675
1500	44.923	124.832	94.960	44.808	-293.536	-203.287	29.619
1600	45.416	127.748	96.919	49.326	-293.534	-197.309	26.951
1700	45.839	130.514	98.815	53.889	-293.550	-191.288	24.591
1800	46.205	133.145	100.649	58.492	-293.592	-185.237	22.491
1900	46.523	135.651	102.425	63.129	-293.665	-179.209	20.614
2000	46.800	138.045	104.147	67.795	-293.773	-173.224	18.929

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 28.911 + 11.352\times10^{-3}T - 10.048\times10^{5}T^{-2}$

$H° - H°_{298} = 28.911\times10^{-3}T + 5.676\times10^{-6}T^{2} + 10.048\times10^{2}T^{-1} - 12.494$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -290.469 - 5.787\times10^{-3}T + 2.217\times10^{-6}T^{2} + 297.250T^{-1}$

$\Delta Gf° = -290.469 + 5.787\times10^{-3}T\ln T - 2.217\times10^{-6}T^{2} + 148.625T^{-1} + 19.039\times10^{-3}T$

Source: Data from JANAF (127) who estimated some molecular constants.

BP(c)
Boron Phosphide
[Formation: $B(\beta) + P(c,l,1/4P_4)(g) = BP(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.248	6.400	6.400	0	-27.600	-26.160	19.176
300	7.260	6.445	6.400	.014	-27.602	-26.150	19.050
317.3	7.376	6.855	6.412	.141	-27.622	-26.065	17.953
317.3	7.376	6.855	6.412	.141	-27.779	-26.065	17.953
400	7.930	8.625	6.693	.773	-27.936	-25.602	13.988
500	8.600	10.467	7.267	1.600	-28.145	-24.991	10.923
550	8.935	11.302	7.597	2.038	-28.255	-24.688	9.810
550	8.935	11.302	7.597	2.038	-31.163	-24.688	9.810
600	9.270	12.094	7.939	2.493	-31.183	-24.098	8.777
700	9.940	13.573	8.639	3.454	-31.212	-22.911	7.153
800	10.610	14.944	9.343	4.481	-31.209	-21.725	5.935
900	11.280	16.233	10.037	5.576	-31.165	-20.541	4.988
1000	11.950	17.456	10.719	6.737	-31.077	-19.365	4.232
1100	12.620	18.626	11.384	7.966	-30.939	-18.205	3.617

Phase changes: 371.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 5.250 + 6.700\times10^{-3}T$
$H°-H°_{298} = 5.250\times10^{-3}T + 3.350\times10^{-6}T^2 - 1.863$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -25.835 - 3.272\times10^{-3}T - 0.527\times10^{-6}T^2 - 221.500T^{-1}$
$\Delta Gf° = -25.835 + 3.272\times10^{-3}T\ln T + 0.527\times10^{-6}T^2 - 110.750T^{-1} - 18.645\times10^{-3}T$
317.30- 550 K: $\Delta Hf° = -25.521 - 5.765\times10^{-3}T + 2.658\times10^{-6}T^2 - 221.500T^{-1}$
$\Delta Gf° = -25.521 + 5.765\times10^{-3}T\ln T - 2.658\times10^{-6}T^2 - 110.750T^{-1} - 32.981\times10^{-3}T$
550-1100 K: $\Delta Hf° = -28.982 - 4.427\times10^{-3}T + 2.654\times10^{-6}T^2 - 321.800T^{-1}$
$\Delta Gf° = -28.982 + 4.427\times10^{-3}T\ln T - 2.654\times10^{-6}T^2 - 160.900T^{-1} - 18.083\times10^{-3}T$

Source: Data from Barin (23).

$BaAl_2O_4(c)$
Barium Aluminate
[Formation: $Ba(c,l) + 2Al(c,l) + 2O_2(g) = BaAl_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	27.175	29.500	29.500	0	-552.400	-523.485	383.720
300	27.359	29.669	29.502	.050	-552.410	-523.306	381.223
400	34.458	38.621	30.673	3.179	-552.623	-513.563	280.594
500	38.692	46.796	33.096	6.850	-552.570	-503.801	220.208
582	41.241	52.867	35.457	10.133	-552.546	-495.801	186.179
600	41.800	54.132	35.999	10.880	-552.467	-494.047	179.954
600	37.566	54.332	35.999	11.000	-552.347	-494.047	179.954
700	38.322	60.180	39.047	14.793	-552.389	-484.331	151.213
768	38.836	63.756	41.078	17.416	-552.499	-477.717	135.942
800	39.078	65.346	42.017	18.663	-552.559	-474.600	129.653
900	39.834	69.993	44.872	22.609	-552.740	-464.845	112.878
933.61	40.088	71.458	45.803	23.952	-552.805	-461.562	108.046
933.61	40.088	71.458	45.803	23.952	-557.965	-461.562	108.046
1000	40.590	74.229	47.599	26.630	-558.045	-454.704	99.374
1002	40.607	74.310	47.652	26.711	-558.048	-454.498	99.131
1002	40.607	74.310	47.652	26.711	-559.900	-454.498	99.131
1100	41.436	78.133	50.199	30.727	-560.016	-444.182	88.250
1200	42.102	81.763	52.681	34.899	-560.049	-433.648	78.977
1300	42.858	85.163	55.050	39.147	-560.002	-423.117	71.132
1400	43.614	88.366	57.315	43.471	-559.894	-412.590	64.407
1500	43.370	91.401	59.488	47.870	-559.723	-402.076	58.582
1600	45.126	94.289	61.573	52.345	-559.490	-391.573	53.486
1700	45.882	97.047	63.579	56.895	-559.192	-381.086	48.991
1800	46.638	99.691	65.513	61.521	-558.830	-370.618	44.999
1900	47.394	102.233	67.379	66.223	-558.404	-360.171	41.429
2000	48.150	104.683	69.183	71.000	-557.913	-349.753	38.219

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
600 K, α - β transition point of $BaAl_2O_4$; ΔH° = 0.120 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 34.199 + 17.732 \times 10^{-3}T - 10.943 \times 10^{5}T^{-2}$
$H° - H°_{298} = 34.199 \times 10^{-3}T + 8.866 \times 10^{-6}T^{2} + 10.943 \times 10^{2}T^{-1} - 14.655$
600-2000 K: $Cp° = 33.030 + 7.560 \times 10^{-3}T$
$H° - H°_{298} = 33.030 \times 10^{-3}T + 3.780 \times 10^{-6}T^{2} - 10.179$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -562.354 + 20.278 \times 10^{-3}T - 13.844 \times 10^{-6}T^{2} + 1532.200T^{-1}$
$\Delta Gf° = -562.354 - 20.278 \times 10^{-3}T\ln T + 13.844 \times 10^{-6}T^{2} + 766.100T^{-1} + 233.157 \times 10^{-3}T$
582-600 K: $\Delta Hf° = -558.833 + 8.038 \times 10^{-3}T - 0.704 \times 10^{-6}T^{2} + 1038.700T^{-1}$
$\Delta Gf° = -558.833 - 8.038 \times 10^{-3}T\ln T + 0.704 \times 10^{-6}T^{2} + 519.350T^{-1} + 157.558 \times 10^{-3}T$
600-768 K: $\Delta Hf° = -554.357 + 6.869 \times 10^{-3}T - 5.790 \times 10^{-6}T^{2} - 55.600T^{-1}$
$\Delta Gf° = -554.357 - 6.869 \times 10^{-3}T\ln T + 5.790 \times 10^{-6}T^{2} - 27.800T^{-1} + 141.088 \times 10^{-3}T$
768-933.61 K: $\Delta Hf° = -551.401 - 1.273 \times 10^{-3}T - 0.199 \times 10^{-6}T^{2} - 56.000T^{-1}$
$\Delta Gf° = -551.401 + 1.273 \times 10^{-3}T\ln T + 0.199 \times 10^{-6}T^{2} - 28.000T^{-1} + 87.439 \times 10^{-3}T$
933.61-1002 K: $\Delta Hf° = -553.937 - 7.269 \times 10^{-3}T + 3.255 \times 10^{-6}T^{2} - 90.800T^{-1}$
$\Delta Gf° = -553.937 + 7.269 \times 10^{-3}T\ln T - 3.255 \times 10^{-6}T^{2} - 45.400T^{-1} + 52.393 \times 10^{-3}T$
1002-2000 K: $\Delta Hf° = -561.191 - 3.202 \times 10^{-3}T + 2.125 \times 10^{-6}T^{2} + 2375.500T^{-1}$
$\Delta Gf° = -561.191 + 3.202 \times 10^{-3}T\ln T - 2.125 \times 10^{-6}T^{2} + 1187.750T^{-1} + 85.374 \times 10^{-3}T$

Source: Data from Fegley (144).

$BaC_2(c)$
Barium Dicarbide
[Formation: $Ba(c,l) + 2C(c) = BaC_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.270	21.000	21.000	0	-18.000	-18.995	13.924
300	15.303	21.095	21.002	.028	-17.992	-19.002	13.842
400	16.516	25.686	21.616	1.628	-17.606	-19.401	10.600
500	17.126	29.444	22.818	3.313	-17.463	-19.874	8.687
582	17.431	32.069	23.941	4.731	-17.617	-20.260	7.608
600	17.498	32.601	24.193	5.045	-17.600	-20.341	7.409
700	17.759	35.319	25.592	6.809	-17.599	-20.802	6.494
768	17.895	36.972	26.528	8.021	-17.687	-21.108	6.007
800	17.959	37.704	26.960	8.595	-17.737	-21.250	5.805
900	18.125	39.829	28.275	10.399	-17.886	-21.683	5.265
1000	18.269	41.747	29.528	12.219	-18.052	-22.097	4.829
1002	18.272	41.784	29.552	12.256	-18.056	-22.105	4.821
1002	18.272	41.784	29.552	12.256	-19.908	-22.105	4.821
1100	18.399	43.494	30.719	14.053	-20.138	-22.286	4.428
1200	18.520	45.100	31.851	15.899	-20.359	-22.494	4.097
1300	18.633	46.587	32.929	17.756	-20.573	-22.663	3.810
1400	18.742	47.972	33.954	19.625	-20.792	-22.818	3.562
1500	18.847	49.269	34.932	21.505	-21.018	-22.953	3.344

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 17.600 + 0.900x10^{-3}T - 2.310x10^{5}T^{-2}$
$H°- H°_{298} = 17.600x10^{-3}T + 0.450x10^{-6}T^{2} + 2.310x10^{2}T^{-1} - 6.062$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -23.604 + 20.287x10^{-3}T - 19.332x10^{-6}T^{2} + 379.900T^{-1}$
$\Delta Gf° = -23.604 - 20.287x10^{-3}T\ln T + 19.332x10^{-6}T^{2} + 189.950T^{-1} + 123.145x10^{-3}T$
582-768 K: $\Delta Hf° = -20.083 + 8.047x10^{-3}T - 6.192x10^{-6}T^{2} - 113.600T^{-1}$
$\Delta Gf° = -20.083 - 8.047x10^{-3}T\ln T + 6.192x10^{-6}T^{2} - 56.800T^{-1} + 47.546x10^{-3}T$
768-1002 K: $\Delta Hf° = -17.128 - 0.095x10^{-3}T - 0.601x10^{-6}T^{2} - 114.000T^{-1}$
$\Delta Gf° = -17.128 + 0.095x10^{-3}T\ln T + 0.601x10^{-6}T^{2} - 57.000T^{-1} - 6.102x10^{-3}T$
1002-1500 K: $\Delta Hf° = -24.382 + 3.972x10^{-3}T - 1.731x10^{-6}T^{2} + 2352.300T^{-1}$
$\Delta Gf° = -24.382 - 3.972x10^{-3}T\ln T + 1.731x10^{-6}T^{2} + 1176.150T^{-1} + 26.879x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Entropy at 298 K from Flowers (153). Other data are those estimated by Barin (23).

$BaCO_3(c)$
Barium Carbonate
[Formation: $Ba(c,l) + C(c) + 1.5O_2(g) = BaCO_3(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H^{o}_{298})/T	H°- H^{o}_{298}	ΔHf°	ΔGf°	
298.15	20.400	26.800	26.800	0	-289.384	-270.601	198.354
300	20.460	26.930	26.803	.038	-289.382	-270.485	197.046
400	23.520	33.280	27.645	2.254	-289.201	-264.213	144.357
500	25.480	38.750	29.334	4.708	-289.068	-257.985	112.764
582	26.800	42.719	30.944	6.853	-289.115	-252.884	94.961
600	27.090	43.540	31.310	7.338	-289.062	-251.764	91.704
700	28.580	47.830	33.369	10.123	-288.784	-245.571	76.670
768	29.546	50.525	34.770	12.099	-288.610	-241.383	68.689
800	30	51.740	35.425	13.052	-288.517	-239.417	65.405
900	31.400	55.350	37.436	16.123	-288.133	-233.298	56.652
1000	32.780	58.730	39.398	19.332	-287.643	-227.231	49.661
1002	32.807	58.796	39.437	19.398	-287.633	-227.110	49.535
1002	32.807	58.796	39.437	19.398	-289.485	-227.110	49.535
1079	33.860	61.400	40.931	22.086	-288.955	-222.346	45.035
1079	37.000	65.290	40.931	26.283	-284.758	-222.346	45.035
1100	37.000	65.970	41.370	27.060	-284.570	-221.097	43.927
1200	37.000	69.190	43.557	30.760	-283.671	-215.378	39.225
1241	37.000	70.510	44.521	32.251	-283.329	-213.171	37.541
1241	38.000	71.110	44.521	32.999	-282.581	-213.171	37.541
1300	38.000	72.770	45.662	35.241	-281.995	-209.746	35.261
1400	38.000	75.590	47.703	39.042	-281.019	-204.232	31.882
1500	38.000	78.210	49.650	42.840	-280.064	-198.779	28.962
1600	38.000	80.660	51.510	46.640	-279.123	-193.386	26.415

Phase changes:
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.
1079 K, α - β transition point of $BaCO_3$; ΔH° = 4.197 kcal/mol.
1241 K, β - γ transition point of $BaCO_3$; ΔH° = 0.748 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1079 K: $Cp^{o} = 20.026 + 13.454\times10^{-3}T - 3.232\times10^{5}T^{-2}$
$H^{o} - H^{o}_{298} = 20.026\times10^{-3}T + 6.727\times10^{-6}T^{2} + 3.232\times10^{2}T^{-1} - 7.653$
1079-1241 K: $Cp^{o} = 152.823 - 68.552\times10^{-3}T - 488.217\times10^{5}T^{-2}$
$H^{o} - H^{o}_{298} = 152.823\times10^{-3}T - 34.276\times10^{-6}T^{2} + 488.217\times10^{2}T^{-1} - 143.955$
1241-1600 K: $Cp^{o} = 36.637 + 0.616\times10^{-3}T + 9.670\times10^{5}T^{-2}$
$H^{o} - H^{o}_{298} = 36.637\times10^{-3}T + 0.308\times10^{-6}T^{2} - 9.670\times10^{2}T^{-1} - 12.163$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf^{o} = -294.746 + 15.386\times10^{-3}T - 13.043\times10^{-6}T^{2} + 576.600T^{-1}$
$\Delta Gf^{o} = -294.746 - 15.386\times10^{-3}T\ln T + 13.043\times10^{-6}T^{2} + 288.300T^{-1} + 161.512\times10^{-3}T$
582-768 K: $\Delta Hf^{o} = -291.225 + 3.146\times10^{-3}T + 0.097\times10^{-6}T^{2} + 83.100T^{-1}$
$\Delta Gf^{o} = -291.225 - 3.146\times10^{-3}T\ln T - 0.097\times10^{-6}T^{2} + 41.550T^{-1} + 85.913\times10^{-3}T$
768-1002 K: $\Delta Hf^{o} = -288.269 - 4.996\times10^{-3}T + 5.688\times10^{-6}T^{2} + 82.700T^{-1}$
$\Delta Gf^{o} = -288.269 + 4.996\times10^{-3}T\ln T - 5.688\times10^{-6}T^{2} + 41.350T^{-1} + 32.265\times10^{-3}T$
1002-1079 K: $\Delta Hf^{o} = -295.523 - 0.929\times10^{-3}T + 4.558\times10^{-6}T^{2} + 2549.000T^{-1}$
$\Delta Gf^{o} = -295.523 + 0.929\times10^{-3}T\ln T - 4.558\times10^{-6}T^{2} + 1274.500T^{-1} + 65.246\times10^{-3}T$

1079-1241 K: $\Delta Hf^{o} = -431.824 - 131.868\times10^{-3}T - 36.445\times10^{-6}T^{2} + 51047.500^{-}1$
$\Delta Gf^{o} = -431.824 + 131.868\times10^{-3}T\ln T + 36.445\times10^{-6}T^{2} + 25523.750T^{-1} + 1053.923\times10^{-3}T$

1241-1600 K: $\Delta Hf^{o} = -300.032 + 15.680\times10^{-3}T - 1.862\times10^{-6}T^{2} + 1258.800^{-}1$
$\Delta Gf^{o} = -300.032 - 15.682\times10^{-3}T\ln T + 1.862\times10^{-6}T^{2} + 629.4000T^{-1} + 179.136\times10^{-3}T$

Source: Data from Chang (74).

$BaFe_2O_4(c)$
Barium Ferrite
[Formation: $Ba(c,l) + 2Fe(c) + 2O_2(g) = BaFe_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	33.140	43.500	43.500	0	-306.000	-281.412	206.278
300	33.289	43.705	43.502	.061	-305.999	-281.259	204.894
400	39.038	54.157	44.887	3.708	-305.750	-273.045	149.183
500	42.503	63.264	47.672	7.796	-305.396	-264.910	115.791
582	44.605	69.883	50.344	11.372	-305.216	-258.285	96.989
600	45.066	71.249	50.951	12.179	-305.112	-256.835	93.551
700	47.205	78.361	54.368	16.795	-304.557	-248.833	77.688
768	48.504	82.798	56.690	20.051	-304.223	-243.439	69.274
800	49.116	84.791	57.775	21.613	-304.071	-240.909	65.813
895	50.809	90.396	60.944	26.360	-303.622	-233.434	57.001
895	49.001	90.536	60.944	26.485	-303.497	-233.434	57.001
900	49.005	90.809	61.109	26.730	-303.485	-233.043	56.590
1000	49.092	95.976	64.341	31.635	-303.478	-225.222	49.222
1002	49.094	96.074	64.404	31.733	-303.486	-225.065	49.089
1002	49.094	96.074	64.404	31.733	-305.338	-225.065	49.089
1043	49.129	98.044	65.688	33.747	-305.647	-221.776	46.470
1100	49.179	100.660	67.434	36.549	-305.778	-217.185	43.150
1161	49.232	103.315	69.250	39.550	-305.702	-212.275	39.959
1161	49.000	104.607	69.250	41.050	-304.202	-212.275	39.959
1185	49.000	105.610	69.976	42.226	-304.154	-210.375	38.799
1185	49.000	105.610	69.976	42.226	-304.584	-210.375	38.799
1200	49.000	106.226	70.425	42.961	-304.495	-209.185	38.097
1300	49.000	110.148	73.332	47.861	-303.918	-201.263	33.835

*Heat capacity at 298 K estimated.

Phase changes:
582 K, α - β transition point of Ba; $\Delta H^\circ = 0$ kcal/mol.
768 K, β - γ transition point of Ba; $\Delta H^\circ = 0$ kcal/mol.
895 K, α - β transition point of $BaFe_2O_4$; $\Delta H^\circ = 0.125$ kcal/mol.
1002 K, melting point of Ba; $\Delta H^\circ = 1.852$ kcal/mol.
1043 K, Curie temperature of Fe; $\Delta H^\circ = 0$ kcal/mol.
1161 K, β - γ transition point of $BaFe_2O_4$; $\Delta H^\circ = 1.500$ kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H^\circ = 0.215$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-895 K: $Cp^\circ = 38.547 + 14.924\times10^{-3}T - 8.765\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 38.547\times10^{-3}T + 7.462\times10^{-6}T^{2} + 8.765\times10^{2}T^{-1} - 15.096$
895-1161 K: $Cp^\circ = 48.224 + 0.868\times10^{-3}T$
$H^\circ - H^\circ_{298} = 48.224\times10^{-3}T + 0.434\times10^{-6}T^{2} - 17.023$
1161-1300 K: $Cp^\circ = 49.000$
$H^\circ - H^\circ_{298} = 49.000\times10^{-3}T - 15.839$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf^\circ = -319.909 + 34.252\times10^{-3}T - 23.936\times10^{-6}T^{2} + 1736.600T^{-1}$
$\Delta Gf^\circ = -319.909 - 34.252\times10^{-3}T\ln T + 23.936\times10^{-6}T^{2} + 868.300T^{-1} + 307.369\times10^{-3}T$
582-768 K: $\Delta Hf^\circ = -316.388 + 22.012\times10^{-3}T - 10.796\times10^{-6}T^{2} + 1243.100T^{-1}$
$\Delta Gf^\circ = -316.388 - 22.012\times10^{-3}T\ln T + 10.796\times10^{-6}T^{2} + 621.550T^{-1} + 231.770\times10^{-3}T$
768-895 K: $\Delta Hf^\circ = -313.432 + 13.870\times10^{-3}T - 5.205\times10^{-6}T^{2} + 1242.700T^{-1}$
$\Delta Gf^\circ = -313.432 - 13.870\times10^{-3}T\ln T + 5.205\times10^{-6}T^{2} + 621.350T^{-1} + 178.122\times10^{-3}T$
895-1002 K: $\Delta Hf^\circ = -315.359 + 23.547\times10^{-3}T - 12.233\times10^{-6}T^{2} + 366.200T^{-1}$
$\Delta Gf^\circ = -315.359 - 23.547\times10^{-3}T\ln T + 12.233\times10^{-6}T^{2} + 183.100T^{-1} + 240.304\times10^{-3}T$
1002-1043 K: $\Delta Hf^\circ = -322.613 + 27.614\times10^{-3}T - 13.363\times10^{-6}T^{2} + 2832.500T^{-1}$
$\Delta Gf^\circ = -322.613 - 27.614\times10^{-3}T\ln T + 13.363\times10^{-6}T^{2} + 1416.250T^{-1} + 273.285\times10^{-3}T$
1043-1161 K: $\Delta Hf^\circ = -275.492 - 60.348\times10^{-3}T + 28.059\times10^{-6}T^{2} + 2375.500T^{-1}$
$\Delta Gf^\circ = -275.492 + 60.348\times10^{-3}T\ln T - 28.059\times10^{-6}T^{2} + 1187.750T^{-1} - 339.804\times10^{-3}T$
1161-1185 K: $\Delta Hf^\circ = -274.308 - 59.572\times10^{-3}T + 27.625\times10^{-6}T^{2} + 2375.500T^{-1}$
$\Delta Gf^\circ = -274.308 + 59.572\times10^{-3}T\ln T - 27.625\times10^{-6}T^{2} + 1187.750T^{-1} - 335.851\times10^{-3}T$
1185-1300 K: $\Delta Hf^\circ = -321.535 + 16.938\times10^{-3}T - 3.757\times10^{-6}T^{2} + 2613.500T^{-1}$
$\Delta Gf^\circ = -321.535 - 16.938\times10^{-3}T\ln T + 3.757\times10^{-6}T^{2} + 1306.750T^{-1} + 208.230\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Massazza (324). Entropy at 298 K based on Deo (120). Heat capacity at 298 K estimated. High-temperature data based on Landiya (296).

$BaH(g)$
Barium Hydride (ideal gas)
[Formation: $Ba(c,l) + 0.5H_2(g) = BaH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.226	52.318	52.318	0	48.646	42.147	-30.894
300	7.232	52.362	52.319	.013	48.640	42.107	-30.675
400	7.567	54.488	52.605	.753	48.307	39.975	-21.841
500	7.883	56.211	53.159	1.526	47.823	37.943	-16.585
582	8.094	57.425	53.678	2.181	47.230	36.365	-13.656
600	8.140	57.672	53.794	2.327	47.159	36.031	-13.124
700	8.341	58.943	54.440	3.152	46.718	34.210	-10.681
768	8.449	59.721	54.874	3.723	46.367	33.012	-9.394
800	8.500	60.067	55.075	3.994	46.201	32.458	-8.867
900	8.627	61.076	55.686	4.851	45.724	30.769	-7.472
1000	8.735	61.991	56.272	5.719	45.261	29.132	-6.367
1002	8.737	62.008	56.283	5.736	45.251	29.099	-6.347
1002	8.737	62.008	56.283	5.736	43.399	29.099	-6.347
1100	8.832	62.828	56.830	6.598	42.904	27.726	-5.508
1200	8.925	63.600	57.362	7.485	42.432	26.366	-4.802
1300	9.021	64.319	57.871	8.383	41.986	25.046	-4.211
1400	9.123	64.991	58.355	9.290	41.546	23.759	-3.709
1500	9.237	65.624	58.819	10.208	41.110	22.505	-3.279
1600	9.364	66.224	59.263	11.138	40.681	21.278	-2.906
1700	9.506	66.796	59.690	12.081	40.261	20.079	-2.581
1800	9.663	67.344	60.100	13.039	39.851	18.901	-2.295
1900	9.834	67.870	60.494	14.014	39.452	17.752	-2.042
2000	10.018	68.380	60.876	15.007	39.068	16.617	-1.816

Phase changes:
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.637 + 1.118\times10^{-3}T - 0.662\times10^{5}T^{-2}$
$H°-H°_{298} = 7.637\times10^{-3}T + 0.559\times10^{-6}T^{2} + 0.662\times10^{2}T^{-1} - 2.549$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = 44.119 + 14.132\times10^{-3}T - 17.900\times10^{-6}T^{2} + 567.950T^{-1}$
$\Delta Gf° = 44.119 - 14.132\times10^{-3}T\ln T + 17.900\times10^{-6}T^{2} + 283.975T^{-1} + 65.374\times10^{-3}T$
582-768 K: $\Delta Hf° = 47.640 + 1.892\times10^{-3}T - 4.760\times10^{-6}T^{2} + 74.450T^{-1}$
$\Delta Gf° = 47.640 - 1.892\times10^{-3}T\ln T + 4.760\times10^{-6}T^{2} + 37.225T^{-1} - 10.225\times10^{-3}T$
768-1002 K: $\Delta Hf° = 50.596 - 6.250\times10^{-3}T + 0.830\times10^{-6}T^{2} + 74.050T^{-1}$
$\Delta Gf° = 50.596 + 6.250\times10^{-3}T\ln T - 0.830\times10^{-6}T^{2} + 37.025T^{-1} - 63.873\times10^{-3}T$
1002-2000 K: $\Delta Hf° = 43.342 - 2.183\times10^{-3}T - 0.300\times10^{-6}T^{2} + 2540.350T^{-1}$
$\Delta Gf° = 43.342 + 2.183\times10^{-3}T\ln T + 0.300\times10^{-6}T^{2} + 1270.175T^{-1} - 30.892\times10^{-3}T$

Source: Data from Gurvich (196).

$BaH_2(c,l)$
Barium Dihydride
[Formation: $Ba(c,l) + H_2(g) = BaH_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	10.994	15.057	15.057	0	-45.430	-36.167	26.511
300	11.007	15.126	15.059	.020	-45.435	-36.110	26.306
400	11.674	18.383	15.498	1.154	-45.721	-32.963	18.010
500	12.342	21.060	16.350	2.355	-46.127	-29.730	12.995
582	12.889	22.975	17.150	3.390	-46.627	-27.004	10.140
600	13.009	23.369	17.331	3.623	-46.674	-26.396	9.615
700	13.677	25.425	18.344	4.957	-46.957	-22.995	7.179
768	14.131	26.713	19.027	5.902	-47.173	-20.656	5.878
800	14.344	27.294	19.347	6.358	-47.268	-19.550	5.341
871	14.818	28.533	20.046	7.392	-47.435	-17.084	4.287
871	16.970	30.071	20.046	8.732	-46.095	-17.084	4.287
900	16.970	30.626	20.377	9.224	-46.092	-16.117	3.914
1000	16.970	32.414	21.493	10.921	-46.085	-12.787	2.795
1002	16.970	32.448	21.515	10.955	-46.086	-12.721	2.775
1002	16.970	32.448	21.515	10.955	-47.938	-12.721	2.775
1100	16.970	34.032	22.561	12.618	-47.986	-9.274	1.842
1200	16.970	35.508	23.579	14.315	-48.016	-5.752	1.048
1300	16.970	36.867	24.550	16.012	-48.036	-2.229	.375
1400	16.970	38.124	25.475	17.709	-48.065	1.295	-.202
1473	16.970	38.987	26.123	18.948	-48.093	3.870	-.574
1473	17.925	43.043	26.123	24.923	-42.118	3.870	-.574
1500	17.925	43.369	26.431	25.407	-42.104	4.713	-.687
1600	17.925	44.526	27.527	27.199	-42.059	7.831	-1.070
1700	17.925	45.612	28.558	28.992	-42.023	10.951	-1.408
1800	17.925	46.637	29.535	30.784	-41.998	14.063	-1.707
1900	17.925	47.606	30.460	32.577	-41.981	17.179	-1.976
2000	17.925	48.526	31.342	34.369	-41.974	20.290	-2.217

Phase changes:
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
871 K, α - β transition point of BaH_2; ΔH° = 1.340 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.
1473 K, melting point of BaH_2; ΔH° = 5.975 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-871 K: $Cp^\circ = 9.031 + 6.634\times10^{-3}T - 0.013\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 9.031\times10^{-3}T + 3.317\times10^{-6}T^2 + 0.013\times10^{2}T^{-1} - 2.992$
871-1473 K: $Cp^\circ = 16.970$
$H^\circ - H^\circ_{298} = 16.970\times10^{-3}T - 6.049$
1473-2000 K: $Cp^\circ = 17.925$
$H^\circ - H^\circ_{298} = 17.925\times10^{-3}T - 1.481$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf^\circ = -49.447 + 12.298\times10^{-3}T - 15.352\times10^{-6}T^2 + 511.300T^{-1}$
$\Delta Gf^\circ = -49.447 - 12.298\times10^{-3}T\ln T + 15.352\times10^{-6}T^2 + 255.650T^{-1} + 107.157\times10^{-3}T$
582-768 K: $\Delta Hf^\circ = -45.926 + 0.058\times10^{-3}T - 2.212\times10^{-6}T^2 + 17.800T^{-1}$
$\Delta Gf^\circ = -45.926 - 0.058\times10^{-3}T\ln T + 2.212\times10^{-6}T^2 + 8.900T^{-1} + 31.557\times10^{-3}T$
768-871 K: $\Delta Hf^\circ = -42.970 - 8.084\times10^{-3}T + 3.379\times10^{-6}T^2 + 17.400T^{-1}$
$\Delta Gf^\circ = -42.970 + 8.084\times10^{-3}T\ln T - 3.379\times10^{-6}T^2 + 8.700T^{-1} - 22.091\times10^{-3}T$
871-1002 K: $\Delta Hf^\circ = -46.027 - 0.145\times10^{-3}T + 0.062\times10^{-6}T^2 + 16.100T^{-1}$
$\Delta Gf^\circ = -46.027 + 0.145\times10^{-3}T\ln T - 0.062\times10^{-6}T^2 + 8.050T^{-1} + 32.275\times10^{-3}T$
1002-1473 K: $\Delta Hf^\circ = -53.281 + 3.922\times10^{-3}T - 1.068\times10^{-6}T^2 + 2482.400T^{-1}$
$\Delta Gf^\circ = -53.281 - 3.922\times10^{-3}T\ln T + 1.068\times10^{-6}T^2 + 1241.200T^{-1} + 65.256\times10^{-3}T$
1473-2000 K: $\Delta Hf^\circ = -48.713 + 4.877\times10^{-3}T - 1.068\times10^{-6}T^2 + 2482.400T^{-1}$
$\Delta Gf^\circ = -48.713 - 4.877\times10^{-3}T\ln T + 1.068\times10^{-6}T^2 + 1241.200T^{-1} + 69.121\times10^{-3}T$

Source: Data from Gurvich (196).

$Ba(IO_3)_2(c)$
Barium Iodate
[Formation: $Ba(c) + I_2(c,l,g) + 3O_2(g) = Ba(IO_3)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	44.800	59.600	59.600	0	-245.500	-206.713	151.523
300	44.900	59.900	59.633	.080	-245.495	-206.481	150.420
386.8	48.893	71.849	61.067	4.171	-245.081	-195.248	110.318
386.8	48.893	71.849	61.067	4.171	-248.790	-195.248	110.318
400	49.500	73.500	61.450	4.820	-248.783	-193.421	105.679
458.4	51.544	80.359	63.397	7.775	-248.720	-185.324	88.355
458.4	51.544	80.359	63.397	7.775	-258.741	-185.324	88.355
500	53.000	84.900	65.000	9.950	-258.272	-178.680	78.100
582	55.624	93.097	68.349	14.404	-257.367	-165.672	62.211
600	56.200	94.800	69.117	15.410	-257.089	-162.840	59.314
700	59.100	103.700	73.457	21.170	-255.477	-147.276	45.981

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 41.735 + 25.900\times10^{-3}T - 4.140\times10^{5}T^{-2}$
$H°-H°_{298} = 41.735\times10^{-3}T + 12.950\times10^{-6}T^2 + 4.140\times10^{2}T^{-1} - 14.983$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -252.387 + 16.891\times10^{-3}T - 8.301\times10^{-6}T^2 + 771.900T^{-1}$
$\Delta Gf° = -252.387 - 16.891\times10^{-3}T\ln T + 8.301\times10^{-6}T^2 + 385.950T^{-1} + 242.612\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -253.842 + 10.487\times10^{-3}T - 6.809\times10^{-6}T^2 + 771.900T^{-1}$
$\Delta Gf° = -253.842 - 10.487\times10^{-3}T\ln T + 6.809\times10^{-6}T^2 + 385.950T^{-1} + 208.797\times10^{-3}T$
458.4-582 K: $\Delta Hf° = -268.555 + 20.827\times10^{-3}T - 6.877\times10^{-6}T^2 + 756.600T^{-1}$
$\Delta Gf° = -268.555 - 20.827\times10^{-3}T\ln T + 6.877\times10^{-6}T^2 + 378.300T^{-1} + 304.260\times10^{-3}T$
582-700 K: $\Delta Hf° = -265.035 + 8.587\times10^{-3}T + 6.263\times10^{-6}T^2 + 263.100T^{-1}$
$\Delta Gf° = -265.035 - 8.587\times10^{-3}T\ln T - 6.263\times10^{-6}T^2 + 131.550T^{-1} + 228.660\times10^{-3}T$

Sources: Data at 298 K from Parker (391). High-temperature data based on Bousquet (54).

$BaMoO_4$(c)
Barium Molydate
[Formation: Ba(c,l) + Mo(c) + $2O_2$(g) = $BaMoO_4$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	28.100	34.500	34.500	0	-369.410	-343.984	252.144
300	28.160	34.670	34.503	.050	-369.409	-343.827	250.474
400	30.600	43.140	35.640	3.000	-369.192	-335.334	183.216
500	32.310	50.160	37.860	6.150	-369.019	-326.890	142.882
582	33.458	55.147	39.949	8.845	-369.031	-319.981	120.156
600	33.710	56.170	40.420	9.450	-368.969	-318.465	115.999
700	34.980	61.470	43.056	12.890	-368.637	-310.073	96.808
768	35.796	64.751	44.844	15.288	-368.443	-304.404	86.623
800	36.180	66.220	45.670	16.440	-368.338	-301.738	82.430
900	37.330	70.540	48.184	20.120	-367.924	-293.425	71.252
1000	38.450	74.540	50.630	23.910	-367.430	-285.182	62.326
1002	38.472	74.617	50.678	23.987	-367.420	-285.018	62.165
1002	38.472	74.617	50.678	23.987	-369.272	-285.018	62.165
1100	39.560	78.250	52.968	27.810	-368.764	-276.792	54.993
1200	40.650	81.740	55.223	31.820	-368.139	-268.459	48.892

*Heat capacities estimated 298 to 683 K.

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 28.169 + 10.570x10^{-3}T - 2.870x10^{5}T^{-2}$
$H°- H°_{298} = 28.169x10^{-3}T + 5.285x10^{-6}T^{2} + 2.870x10^{2}T^{-1} - 9.831$

Formation equations (kcal/mol):

298.15-582 K: $ΔHf° = -376.257 + 19.055x10^{-3}T - 15.156x10^{-6}T^{2} + 749.300T^{-1}$
$ΔGf° = -376.257 - 19.055x10^{-3}TlnT + 15.156x10^{-6}T^{2} + 374.650T^{-1} + 208.078x10^{-3}T$
582-768 K: $ΔHf° = -372.736 + 6.815x10^{-3}T - 2.016x10^{-6}T^{2} + 255.800T^{-1}$
$ΔGf° = -372.736 - 6.815x10^{-3}TlnT + 2.016x10^{-6}T^{2} + 127.900T^{-1} + 132.479x10^{-3}T$
768-1002 K: $ΔHf° = -369.781 - 1.327x10^{-3}T + 3.575x10^{-6}T^{2} + 255.400T^{-1}$
$ΔGf° = -369.781 + 1.327x10^{-3}TlnT - 3.575x10^{-6}T^{2} + 127.700T^{-1} + 78.830x10^{-3}T$
1002-1200 K: $ΔHf° = -377.035 + 2.740x10^{-3}T + 2.445x10^{-6}T^{2} + 2721.700T^{-1}$
$ΔGf° = -377.035 - 2.740x10^{-3}TlnT - 2.445x10^{-6}T^{2} + 1360.850T^{-1} + 111.811x10^{-3}T$

Sources: Enthalpy of formation at 298 K from O'Hare (362). Entropy at 298 K from Kubaschewski (288). High-temperature data based on Zharkova (543). Heat capacities estimated 298 to 683 K.

Ba_3N_2(c)
Tribarium Dinitride
[Formation: $3Ba(c) + N_2(g) = Ba_3N_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	28.007	36.400	36.400	0	-86.800	-70.663	51.797
300	28.050	36.573	36.400	.052	-86.797	-70.561	51.403
400	30.400	44.965	37.530	2.974	-86.750	-65.170	35.607
500	32.750	52.001	39.737	6.132	-87.019	-59.755	26.118
582	34.677	57.117	41.832	8.896	-87.722	-55.236	20.742
600	35.100	58.180	42.307	9.524	-87.685	-54.231	19.753
700	37.450	63.767	44.978	13.152	-87.529	-48.669	15.195
768	39.048	67.312	46.801	15.752	-87.478	-44.895	12.776
800	39.800	68.921	47.653	17.014	-87.428	-43.122	11.780
900	42.150	73.744	50.286	21.112	-87.026	-37.605	9.132
950	43.325	76.055	51.583	23.248	-86.730	-34.869	8.022

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-950 K: $Cp° = 21.000 + 23.500\times10^{-3}T$
$H° - H°_{298} = 21.000\times10^{-3}T + 11.750\times10^{-6}T^2 - 7.306$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -100.932 + 43.652\times10^{-3}T - 43.589\times10^{-6}T^2 + 1488.400T^{-1}$
$\Delta Gf° = -100.932 - 43.652\times10^{-3}T\ln T + 43.589\times10^{-6}T^2 + 744.200T^{-1} + 328.867\times10^{-3}T$
582-768 K: $\Delta Hf° = -90.370 + 6.932\times10^{-3}T - 4.169\times10^{-6}T^2 + 7.900T^{-1}$
$\Delta Gf° = -90.370 - 6.932\times10^{-3}T\ln T + 4.169\times10^{-6}T^2 + 3.950T^{-1} + 102.070\times10^{-3}T$
768-950 K: $\Delta Hf° = -81.502 - 17.494\times10^{-3}T + 12.604\times10^{-6}T^2 + 6.700T^{-1}$
$\Delta Gf° = -81.502 + 17.494\times10^{-3}T\ln T - 12.604\times10^{-6}T^2 + 3.350T^{-1} - 58.875\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Other data are those estimated by Barin (23).

$Ba(NO_3)_2(c)$
Barium Nitrate
[Formation: $Ba(c,l) + N_2(g) + 3O_2(g) = Ba(NO_3)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	36.290	51.100	51.100	0	-237.110	-190.419	139.579
300	36.400	51.320	51.100	.070	-237.104	-190.124	138.503
400	41.700	62.550	52.600	3.980	-236.747	-174.519	95.352
500	46.190	72.350	55.590	8.380	-236.151	-159.027	69.510
582	49.609	79.618	58.466	12.310	-235.617	-146.418	54.981
600	50.360	81.140	59.123	13.210	-235.414	-143.662	52.328
700	54.370	89.210	62.853	18.450	-234.150	-128.467	40.109
768	57.042	94.376	65.425	22.235	-233.174	-118.254	33.651
800	58.300	96.730	66.630	24.080	-232.663	-113.477	31.000
850	60.250	100.320	68.496	27.050	-231.777	-106.044	27.265

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-850 K: $Cp° = 28.527 + 37.832 \times 10^{-3}T - 3.131 \times 10^{5}T^{-2}$
$H° - H°_{298} = 28.527 \times 10^{-3}T + 18.916 \times 10^{-6}T^{2} + 3.131 \times 10^{2}T^{-1} - 11.237$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -242.254 + 10.043 \times 10^{-3}T - 1.432 \times 10^{-6}T^{2} + 678.900T^{-1}$
$\Delta Gf° = -242.254 - 10.043 \times 10^{-3}T\ln T + 1.432 \times 10^{-6}T^{2} + 339.450T^{-1} + 226.832 \times 10^{-3}T$
582-768 K: $\Delta Hf° = -238.733 - 2.197 \times 10^{-3}T + 11.708 \times 10^{-6}T^{2} + 185.400T^{-1}$
$\Delta Gf° = -238.733 + 2.197 \times 10^{-3}T\ln T - 11.708 \times 10^{-6}T^{2} + 92.700T^{-1} + 151.233 \times 10^{-3}T$
768-850 K: $\Delta Hf° = -235.777 - 10.339 \times 10^{-3}T + 17.299 \times 10^{-6}T^{2} + 185.000T^{-1}$
$\Delta Gf° = -235.777 + 10.339 \times 10^{-3}T\ln T - 17.299 \times 10^{-6}T^{2} + 92.500T^{-1} + 97.584 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Shomate (454). High-temperature data based on Shomate (450).

$BaOH(g)$
Barium Monohydroxide (ideal gas)
[Formation: $Ba(c,l) + 0.5H_2(g) + 0.5O_2(g) = BaOH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.079	60.416	60.416	0	-54.120	-55.728	40.849
300	11.097	60.485	60.416	.021	-54.124	-55.737	40.604
400	11.797	63.784	60.861	1.169	-54.404	-56.237	30.726
500	12.174	66.461	61.723	2.369	-54.827	-56.652	24.762
582	12.366	68.326	62.525	3.376	-55.377	-56.911	21.371
600	12.408	68.703	62.705	3.599	-55.439	-56.957	20.746
700	12.581	70.629	63.702	4.849	-55.845	-57.179	17.852
768	12.683	71.800	64.368	5.708	-56.177	-57.293	16.304
800	12.731	72.319	64.675	6.115	-56.337	-57.337	15.664
900	12.871	73.827	65.610	7.395	-56.798	-57.435	13.947
1000	13.008	75.190	66.501	8.689	-57.249	-57.482	12.562
1002	13.011	75.216	66.518	8.715	-57.258	-57.482	12.537
1002	13.011	75.216	66.518	8.715	-59.110	-57.482	12.537
1100	13.141	76.436	67.349	9.996	-59.596	-57.299	11.384
1200	13.269	77.585	68.154	11.317	-60.058	-57.069	10.394
1300	13.391	78.652	68.921	12.650	-60.497	-56.802	9.549
1400	13.507	79.648	69.652	13.995	-60.932	-56.502	8.820
1500	13.615	80.584	70.350	15.351	-61.365	-56.170	8.184
1600	13.718	81.466	71.017	16.718	-61.795	-55.810	7.623
1700	13.816	82.301	71.657	18.095	-62.222	-55.422	7.125
1800	13.910	83.093	72.270	19.481	-62.649	-55.010	6.679
1900	14.000	83.848	72.861	20.876	-63.074	-54.575	6.277
2000	14.089	84.568	73.427	22.281	-63.496	-54.116	5.913

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.139 + 1.008\times10^{-3}T - 1.209\times10^{5}T^{-2}$
$H°- H°_{298} = 12.139\times10^{-3}T + 0.504\times10^{-6}T^{2} + 1.209\times10^{2}T^{-1} - 4.070$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -58.992 + 15.019\times10^{-3}T - 18.207\times10^{-6}T^{2} + 600.050T^{-1}$
$\Delta Gf° = -58.992 - 15.019\times10^{-3}T\ln T + 18.207\times10^{-6}T^{2} + 300.025T^{-1} + 87.717\times10^{-3}T$
582-768 K: $\Delta Hf° = -55.471 + 2.779\times10^{-3}T - 5.067\times10^{-6}T^{2} + 106.550T^{-1}$
$\Delta Gf° = -55.471 - 2.779\times10^{-3}T\ln T + 5.067\times10^{-6}T^{2} + 53.275T^{-1} + 12.118\times10^{-3}T$
768-1002 K: $\Delta Hf° = -52.515 - 5.363\times10^{-3}T + 0.524\times10^{-6}T^{2} + 106.150T^{-1}$
$\Delta Gf° = -52.515 + 5.363\times10^{-3}T\ln T - 0.524\times10^{-6}T^{2} + 53.075T^{-1} - 41.530\times10^{-3}T$
1002-2000 K: $\Delta Hf° = -59.769 - 1.296\times10^{-3}T - 0.606\times10^{-6}T^{2} + 2572.450T^{-1}$
$\Delta Gf° = -59.769 + 1.296\times10^{-3}T\ln T + 0.606\times10^{-6}T^{2} + 1286.225T^{-1} - 8.549\times10^{-3}T$

Source: Data from Chase (82) who estimated all except enthalpy of formation at 298 K.

$Ba(OH)_2(c,l)$
Barium Dihydroxide
[Formation: $Ba(c,l) + H_2(g) + O_2(g) = Ba(OH)_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	24.290	25.600	25.600	0	-226.170	-205.440	150.589
300	24.330	25.750	25.600	.045	-226.163	-205.310	149.567
400	26.920	33.145	26.590	2.622	-225.716	-198.426	108.414
500	28.360	39.321	28.537	5.392	-225.284	-191.657	83.772
582	29.155	43.686	30.371	7.750	-225.079	-186.161	69.905
600	29.330	44.577	30.784	8.276	-224.970	-184.958	67.370
681	30.120	48.337	32.648	10.684	-224.489	-179.586	57.633
681	33.700	54.211	32.648	14.684	-220.489	-179.586	57.633
700	33.700	55.138	33.247	15.324	-220.317	-178.447	55.713
768	33.700	58.262	35.325	17.616	-219.728	-174.408	49.631
800	33.700	59.638	36.271	18.694	-219.457	-172.526	47.131
900	33.700	63.608	39.092	22.064	-218.591	-166.712	40.483
1000	33.700	67.158	41.724	25.434	-217.738	-160.994	35.185
1002	33.700	67.225	41.775	25.501	-217.722	-160.881	35.090
1002	33.700	67.225	41.775	25.501	-219.574	-160.881	35.090
1100	33.700	70.370	44.185	28.804	-218.805	-155.175	30.830
1200	33.700	73.303	46.491	32.174	-218.010	-149.426	27.214
1300	33.700	76.000	48.658	35.544	-217.213	-143.742	24.165
1400	33.700	78.498	50.702	38.914	-216.433	-138.123	21.562

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
681 K, melting point of $Ba(OH)_2$; ΔH° = 4.000 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-681 K: $Cp° = 27.316 + 5.334\times10^{-3}T - 4.104\times10^{5}T^{-2}$
$H°-H°_{298} = 27.316\times10^{-3}T + 2.667\times10^{-6}T^{2} + 4.104\times10^{2}T^{-1} - 9.758$
681-1400 K: $Cp° = 33.700$
$H°-H°_{298} = 33.700\times10^{-3}T - 8.266$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -234.601 + 23.353\times10^{-3}T - 16.505\times10^{-6}T^{2} + 875.200T^{-1}$
$\Delta Gf° = -234.601 - 23.353\times10^{-3}T\ln T + 16.505\times10^{-6}T^{2} + 437.600T^{-1} + 221.020\times10^{-3}T$
582-681 K: $\Delta Hf° = -231.080 + 11.113\times10^{-3}T - 3.365\times10^{-6}T^{2} + 381.700T^{-1}$
$\Delta Gf° = -231.080 - 11.113\times10^{-3}T\ln T + 3.365\times10^{-6}T^{2} + 190.850T^{-1} + 145.421\times10^{-3}T$
681-768 K: $\Delta Hf° = -229.588 + 17.497\times10^{-3}T - 6.032\times10^{-6}T^{2} - 28.700T^{-1}$
$\Delta Gf° = -229.588 - 17.497\times10^{-3}T\ln T + 6.032\times10^{-6}T^{2} - 14.350T^{-1} + 183.503\times10^{-3}T$
768-1002 K: $\Delta Hf° = -226.632 + 9.355\times10^{-3}T - 0.441\times10^{-6}T^{2} - 29.100T^{-1}$
$\Delta Gf° = -226.632 - 9.355\times10^{-3}T\ln T + 0.441\times10^{-6}T^{2} - 14.550T^{-1} + 129.854\times10^{-3}T$
1002-1400 K: $\Delta Hf° = -233.886 + 13.422\times10^{-3}T - 1.571\times10^{-6}T^{2} + 2437.200T^{-1}$
$\Delta Gf° = -233.886 - 13.422\times10^{-3}T\ln T + 1.571\times10^{-6}T^{2} + 1218.600T^{-1} + 162.835\times10^{-3}T$

Source: Data from Chase (82).

$Ba(OH)_2(g)$
Barium Dihydroxide (ideal gas)
[Formation: $Ba(c,l) + H_2(g) + O_2(g) = Ba(OH)_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.464	75.263	75.263	0	-149.750	-143.827	105.426
300	18.498	75.378	75.265	.034	-149.754	-143.790	104.749
400	19.809	80.901	76.008	1.957	-149.961	-141.774	77.461
500	20.506	85.403	77.451	3.976	-150.280	-139.694	61.059
582	20.860	88.545	78.797	5.674	-150.734	-137.924	51.792
600	20.938	89.182	79.099	6.050	-150.776	-137.527	50.094
700	21.261	92.435	80.778	8.160	-151.061	-135.299	42.242
768	21.453	94.415	81.898	9.613	-151.311	-133.756	38.063
800	21.544	95.293	82.417	10.301	-151.430	-133.023	36.340
900	21.814	97.846	83.992	12.469	-151.766	-130.702	31.738
1000	22.079	100.158	85.495	14.663	-152.089	-128.345	28.049
1002	22.084	100.202	85.524	14.707	-152.096	-128.297	27.983
1002	22.084	100.202	85.524	14.707	-153.948	-128.297	27.983
1100	22.338	102.275	86.926	16.884	-154.305	-125.771	24.988
1200	22.589	104.229	88.286	19.131	-154.633	-123.161	22.430
1300	22.827	106.047	89.584	21.402	-154.935	-120.525	20.262
1400	23.051	107.747	90.821	23.696	-155.231	-117.869	18.400
1500	23.259	109.344	92.003	26.011	-155.523	-115.189	16.783
1600	23.452	110.852	93.135	28.347	-155.811	-112.493	15.366
1700	23.629	112.279	94.220	30.701	-156.096	-109.774	14.112
1800	23.790	113.634	95.261	33.072	-156.380	-107.042	12.997
1900	23.938	114.924	96.261	35.459	-156.663	-104.291	11.996
2000	24.073	116.156	97.227	37.859	-156.947	-101.531	11.095

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 20.368 + 1.964\text{x}10^{-3}T - 2.213\text{x}10^{5}T^{-2}$
$H°- H°_{298} = 20.368\text{x}10^{-3}T + 0.982\text{x}10^{-6}T^2 + 2.213\text{x}10^{2}T^{-1} - 6.902$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -155.325 + 16.405\text{x}10^{-3}T - 18.190\text{x}10^{-6}T^2 + 686.100T^{-1}$
$\Delta Gf° = -155.325 - 16.405\text{x}10^{-3}T\ln T + 18.190\text{x}10^{-6}T^2 + 343.050T^{-1} + 122.753\text{x}10^{-3}T$
582-768 K: $\Delta Hf° = -151.805 + 4.165\text{x}10^{-3}T - 5.050\text{x}10^{-6}T^2 + 192.600T^{-1}$
$\Delta Gf° = -151.805 - 4.165\text{x}10^{-3}T\ln T + 5.050\text{x}10^{-6}T^2 + 96.300T^{-1} + 47.154\text{x}10^{-3}T$
768-1002 K: $\Delta Hf° = -148.849 - 3.977\text{x}10^{-3}T + 0.541\text{x}10^{-6}T^2 + 192.200T^{-1}$
$\Delta Gf° = -148.849 + 3.977\text{x}10^{-3}T\ln T - 0.541\text{x}10^{-6}T^2 + 96.100T^{-1} - 6.494\text{x}10^{-3}T$
1002-2000 K: $\Delta Hf° = -156.103 + 0.090\text{x}10^{-3}T - 0.589\text{x}10^{-6}T^2 + 2658.500T^{-1}$
$\Delta Gf° = -156.103 - 0.090\text{x}10^{-3}T\ln T + 0.589\text{x}10^{-6}T^2 + 1329.250T^{-1} + 26.487\text{x}10^{-3}T$

Source: Data from Chase (82).

$BaSO_4$(c)
Barium Sulfate
[Reaction: $Ba(c,l) + 0.5S_2(g) + 2O_2(g) = BaSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	24.414	31.600	31.600	0	-367.555	-335.182	245.692
300*	24.537	31.749	31.602	.044	-367.556	-334.980	244.030
400	28.387	39.356	32.608	2.699	-367.446	-324.135	177.097
500	30.380	45.929	34.633	5.648	-367.281	-313.327	136.953
582	31.270	50.618	36.562	8.180	-367.291	-304.481	114.336
600	31.465	51.573	36.998	8.745	-367.233	-302.539	110.198
700	32.120	56.476	39.437	11.927	-366.952	-291.779	91.096
768	32.409	59.469	41.080	14.123	-366.816	-284.485	80.955
800	32.545	60.795	41.842	15.162	-366.755	-281.056	76.780
900	32.836	64.646	44.166	18.432	-366.531	-270.357	65.651
1000	33.043	68.117	46.391	21.726	-366.307	-259.684	56.753
1002	33.046	68.183	46.434	21.792	-366.303	-259.470	56.593
1002	33.046	68.183	46.434	21.792	-368.155	-259.470	56.593
1100	33.194	71.273	48.511	25.038	-367.993	-248.846	49.441
1200	33.308	74.167	50.530	28.364	-367.805	-238.023	43.349
1300	33.394	76.836	52.452	31.699	-367.607	-227.215	38.198

*Data extrapolated 298 to 500 K.

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp° = 33.095 + 0.760 \times 10^{-3}T - 7.918 \times 10^{5}T^{-2}$
$H°-H°_{298} = 33.095 \times 10^{-3}T + 0.380 \times 10^{-6}T^{2} + 7.918 \times 10^{2}T^{-1} - 12.557$

Reaction equations (kcal/mol):

298.15-582 K: $\Delta Hr° = -376.967 + 24.187 \times 10^{-3}T - 19.036 \times 10^{-6}T^{2} + 1160.750T^{-1}$
$\Delta Gr° = -376.967 - 24.187 \times 10^{-3}T\ln T + 19.036 \times 10^{-6}T^{2} + 580.375T^{-1} + 265.750 \times 10^{-3}T$
582-768 K: $\Delta Hr° = -373.446 + 11.947 \times 10^{-3}T - 5.896 \times 10^{-6}T^{2} + 667.250T^{-1}$
$\Delta Gr° = -373.446 - 11.947 \times 10^{-3}T\ln T + 5.896 \times 10^{-6}T^{2} + 333.625T^{-1} + 190.151 \times 10^{-3}T$
768-1002 K: $\Delta Hr° = -370.491 + 3.805 \times 10^{-3}T - 0.305 \times 10^{-6}T^{2} + 666.850T^{-1}$
$\Delta Gr° = -370.491 - 3.805 \times 10^{-3}T\ln T + 0.305 \times 10^{-6}T^{2} + 333.425T^{-1} + 136.503 \times 10^{-3}T$
1002-1300 K: $\Delta Hr° = -377.745 + 7.872 \times 10^{-3}T - 1.435 \times 10^{-6}T^{2} + 3133.150T^{-1}$
$\Delta Gr° = -377.745 - 7.872 \times 10^{-3}T\ln T + 1.435 \times 10^{-6}T^{2} + 1566.575T^{-1} + 169.484 \times 10^{-3}T$

Source: Data from DeKock (113) who extrapolated 298 to 500 K.

$BaSiO_3(c)$
Barium Metasilicate
[Formation: $Ba(c,l) + Si(c,l) + 1.5O_2(g) = BaSiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	21.462	26.200	26.200	0	-388.050	-368.156	269.862
300*	21.540	26.333	26.200	.040	-388.050	-368.031	268.107
400	24.430	32.975	27.087	2.355	-388.033	-361.365	197.438
500	26.022	38.611	28.843	4.884	-388.055	-354.696	155.035
582	26.908	42.633	30.508	7.057	-388.237	-349.214	131.134
600	27.103	43.456	30.884	7.543	-388.215	-348.007	126.760
700	27.944	47.700	32.990	10.297	-388.134	-341.314	106.562
768	28.427	50.314	34.409	12.215	-388.120	-336.766	95.832
800	28.655	51.479	35.069	13.128	-388.112	-334.627	91.415
900	29.292	54.891	37.084	16.026	-388.033	-327.945	79.635
1000	29.883	58.008	39.023	18.985	-387.915	-321.266	70.212
1002	29.894	58.068	39.061	19.045	-387.913	-321.133	70.043
1002	29.894	58.068	39.061	19.045	-389.765	-321.133	70.043
1100	30.443	60.883	40.882	22.001	-389.666	-314.432	62.471
1200	30.983	63.555	42.661	25.073	-389.501	-307.599	56.021
1300	31.508	66.056	44.366	28.197	-389.283	-300.783	50.566
1400	32.022	68.410	46.000	31.374	-389.029	-293.982	45.892
1500	32.529	70.636	47.569	34.601	-388.739	-287.213	41.846
1600	33.030	72.752	49.078	37.879	-388.415	-280.457	38.308
1687	33.462	74.512	50.344	40.772	-388.103	-274.573	35.570
1687	33.462	74.512	50.344	40.772	-400.185	-274.573	35.570
1700	33.526	74.769	50.530	41.207	-400.127	-273.601	35.173
1800	34.019	76.699	51.930	44.584	-399.662	-266.169	32.317
1900	34.508	78.552	53.283	48.011	-399.156	-258.766	29.764
2000	34.996	80.334	54.591	51.486	-398.609	-251.397	27.471

*Data above 298 K estimated.

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.643 + 4.738\times10^{-3}T - 4.972\times10^{5}T^{-2}$
$H°-H°_{298} = 25.643\times10^{-3}T + 2.369\times10^{-6}T^{2} + 4.972\times10^{2}T^{-1} - 9.524$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -394.923 + 18.842\times10^{-3}T - 16.986\times10^{-6}T^{2} + 824.400T^{-1}$
$\Delta Gf° = -394.923 - 18.842\times10^{-3}T\ln T + 16.986\times10^{-6}T^{2} + 412.200T^{-1} + 187.430\times10^{-3}T$
582-768 K: $\Delta Hf° = -391.402 + 6.602\times10^{-3}T - 3.846\times10^{-6}T^{2} + 330.900T^{-1}$
$\Delta Gf° = -391.402 - 6.602\times10^{-3}T\ln T + 3.846\times10^{-6}T^{2} + 165.450T^{-1} + 111.830\times10^{-3}T$
768-1002 K: $\Delta Hf° = -388.446 - 1.540\times10^{-3}T + 1.745\times10^{-6}T^{2} + 330.500T^{-1}$
$\Delta Gf° = -388.446 + 1.540\times10^{-3}T\ln T - 1.745\times10^{-6}T^{2} + 165.250T^{-1} + 58.182\times10^{-3}T$
1002-1687 K: $\Delta Hf° = -395.700 + 2.527\times10^{-3}T + 0.615\times10^{-6}T^{2} + 2796.800T^{-1}$
$\Delta Gf° = -395.700 - 2.527\times10^{-3}T\ln T - 0.615\times10^{-6}T^{2} + 1398.400T^{-1} + 91.163\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -408.129 + 2.106\times10^{-3}T + 0.966\times10^{-6}T^{2} + 2895.300T^{-1}$
$\Delta Gf° = -408.129 - 2.106\times10^{-3}T\ln T - 0.966\times10^{-6}T^{2} + 1447.650T^{-1} + 95.977\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 from Weller (521). High-temperature data are those estimated by Fegley (144).

$Ba_2SiO_4(c)$
Barium Orthosilicate
[Formation: $2Ba(c,l) + Si(c,l) + 2O_2(g) = Ba_2SiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	32.229	42.100	42.100	0	-546.800	-519.893	381.087
300*	32.343	42.300	42.100	.060	-546.799	-519.725	378.614
400	36.583	52.258	43.431	3.531	-546.707	-510.721	279.041
500	38.912	60.692	46.062	7.315	-546.747	-501.724	219.301
582	40.205	66.704	48.555	10.563	-547.123	-494.317	185.621
600	40.489	67.933	49.118	11.289	-547.085	-492.684	179.458
700	41.710	74.270	52.269	15.401	-546.950	-483.631	150.994
768	42.412	78.170	54.391	18.263	-546.944	-477.479	135.875
800	42.742	79.908	55.377	19.625	-546.939	-474.585	129.649
900	43.664	84.997	58.390	23.946	-546.824	-465.548	113.049
1000	44.518	89.642	61.286	28.356	-546.640	-456.518	99.771
1002	44.534	89.731	61.343	28.445	-546.637	-456.338	99.532
1002	44.534	89.731	61.343	28.445	-550.341	-456.338	99.532
1100	45.327	93.923	64.061	32.848	-550.207	-447.156	88.840
1200	46.106	97.900	66.717	37.420	-549.957	-437.798	79.733
1300	46.863	101.621	69.260	42.069	-549.612	-428.464	72.030
1400	47.604	105.121	71.698	46.792	-549.214	-419.158	65.433
1500	48.335	108.430	74.037	51.589	-548.760	-409.893	59.721
1600	49.056	111.573	76.286	56.459	-548.252	-400.654	54.726
1687	49.678	114.186	78.174	60.754	-547.765	-392.618	50.863
1687	49.678	114.186	78.174	60.754	-559.847	-392.618	50.863
1700	49.771	114.568	78.450	61.400	-559.762	-391.326	50.308
1800	50.480	117.433	80.537	66.412	-559.076	-381.436	46.312
1900	51.185	120.181	82.552	71.496	-558.330	-371.585	42.741
2000	51.887	122.825	84.500	76.649	-557.525	-361.787	39.534

*Data above 298 K estimated.

Phase changes:
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 38.432 + 6.818\times10^{-3}T - 7.321\times10^{5}T^{-2}$
$H° - H°_{298} = 38.432\times10^{-3}T + 3.409\times10^{-6}T^{2} + 7.321\times10^{2}T^{-1} - 14.217$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -560.122 + 37.739\times10^{-3}T - 34.448\times10^{-6}T^{2} + 1530.200T^{-1}$
$\Delta Gf° = -560.122 - 37.739\times10^{-3}T\ln T + 34.448\times10^{-6}T^{2} + 765.100T^{-1} + 331.072\times10^{-3}T$
582-768 K: $\Delta Hf° = -553.080 + 13.259\times10^{-3}T - 8.168\times10^{-6}T^{2} + 543.200T^{-1}$
$\Delta Gf° = -553.080 - 13.259\times10^{-3}T\ln T + 8.168\times10^{-6}T^{2} + 271.600T^{-1} + 179.874\times10^{-3}T$
768-1002 K: $\Delta Hf° = -547.169 - 3.025\times10^{-3}T + 3.014\times10^{-6}T^{2} + 542.400T^{-1}$
$\Delta Gf° = -547.169 + 3.025\times10^{-3}T\ln T - 3.014\times10^{-6}T^{2} + 271.200T^{-1} + 72.577\times10^{-3}T$
1002-1687 K: $\Delta Hf° = -561.677 + 5.109\times10^{-3}T + 0.754\times10^{-6}T^{2} + 5475.000T^{-1}$
$\Delta Gf° = -561.677 - 5.109\times10^{-3}T\ln T - 0.754\times10^{-6}T^{2} + 2737.500T^{-1} + 138.539\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -574.106 + 4.688\times10^{-3}T + 1.105\times10^{-6}T^{2} + 5573.500T^{-1}$
$\Delta Gf° = -574.106 - 4.688\times10^{-3}T\ln T - 1.105\times10^{-6}T^{2} + 2786.750T^{-1} + 143.353\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Weller (521). High-temperature data are those estimated by Fegley (144).

$BaTiO_3(c)$
Barium Metatitanate
[Formation: $Ba(c,l) + Ti(c) + 1.5O_2(g) = BaTiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.490	25.800	25.800	0	-396.700	-375.846	275.499
300	24.497	25.951	25.801	.045	-396.698	-375.715	273.704
350	25.782	29.816	26.102	1.300	-396.621	-372.226	232.425
398	30.979	33.345	26.762	2.620	-396.480	-368.887	202.561
398	27.564	33.345	26.762	2.620	-396.480	-368.887	202.561
400	27.576	33.483	26.796	2.675	-396.475	-368.749	201.472
500	28.170	39.701	28.775	5.463	-396.334	-361.840	158.158
582	28.625	44.013	30.625	7.792	-396.435	-356.177	133.748
600	28.725	44.886	31.039	8.308	-396.401	-354.932	129.282
700	29.242	49.354	33.344	11.207	-396.273	-348.027	108.658
768	29.567	52.080	34.884	13.206	-396.249	-343.344	97.704
800	29.720	53.290	35.596	14.155	-396.241	-341.141	93.194
900	30.159	56.816	37.762	17.149	-396.185	-334.255	81.167
1000	30.559	60.015	39.830	20.185	-396.119	-327.377	71.547
1002	30.566	60.076	39.870	20.246	-396.118	-327.239	71.374
1002	30.566	60.076	39.870	20.246	-397.970	-327.239	71.374
1100	30.921	62.945	41.800	23.260	-397.957	-320.327	63.642
1156	31.102	64.485	42.861	24.996	-397.938	-316.372	59.812
1156	31.102	64.485	42.861	24.996	-398.955	-316.372	59.812
1200	31.244	65.649	43.676	26.368	-398.888	-313.230	57.046
1300	31.528	68.162	45.464	29.507	-398.725	-306.099	51.459
1400	31.774	70.508	47.170	32.673	-398.566	-298.981	46.673
1500	31.981	72.707	48.800	35.861	-398.413	-291.871	42.525
1600	32.149	74.777	50.360	39.068	-398.273	-284.775	38.898
1700	32.279	76.730	51.854	42.289	-398.151	-277.684	35.698
1800	32.370	78.577	53.287	45.522	-398.056	-270.600	32.855

Phase changes:
398 K, Curie temperature of $BaTiO_3$; ΔH° = 0 kcal/mol.
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-398 K: $Cp° = - 31.552 + 126.754\times10^{-3}T + 16.224\times10^{5}T^{-2}$
$H° - H°_{298} = - 31.552\times10^{-3}T + 63.377\times10^{-6}T^{2} - 16.224\times10^{2}T^{-1} + 9.215$
398-1800 K: $Cp° = 27.124 + 3.432\times10^{-3}T - 1.467\times10^{5}T^{-2}$
$H° - H°_{298} = 27.124\times10^{-3}T + 1.716\times10^{-6}T^{2} + 1.467\times10^{2}T^{-1} - 8.816$

Formation equations (kcal/mol):

298.15-398 K: $\Delta Hf° = -385.107 - 38.151\times10^{-3}T + 43.250\times10^{-6}T^{2} - 1211.500T^{-1}$
$\Delta Gf° = -385.107 + 38.151\times10^{-3}T\ln T - 43.250\times10^{-6}T^{2} - 605.750T^{-1} - 166.599\times10^{-3}T$
398-582 K: $\Delta Hf° = -403.137 + 20.525\times10^{-3}T - 18.411\times10^{-6}T^{2} + 557.600T^{-1}$
$\Delta Gf° = -403.137 - 20.525\times10^{-3}T\ln T + 18.411\times10^{-6}T^{2} + 278.800T^{-1} + 199.840\times10^{-3}T$
582-768 K: $\Delta Hf° = -399.616 + 8.285\times10^{-3}T - 5.271\times10^{-6}T^{2} + 64.100T^{-1}$
$\Delta Gf° = -399.616 - 8.285\times10^{-3}T\ln T + 5.271\times10^{-6}T^{2} + 32.050T^{-1} + 124.241\times10^{-3}T$
768-1002 K: $\Delta Hf° = -396.661 + 0.143\times10^{-3}T + 0.319\times10^{-6}T^{2} + 63.700T^{-1}$
$\Delta Gf° = -396.661 - 0.143\times10^{-3}T\ln T - 0.319\times10^{-6}T^{2} + 31.850T^{-1} + 70.593\times10^{-3}T$

1002-1156 K: $\Delta Hf° = -403.915 + 4.210\times10^{-3}T - 0.811\times10^{-6}T^{2} + 2530.000^{-}1$
$\Delta Gf° = -403.915 - 4.210\times10^{-3}T\ln T + 0.811\times10^{-6}T^{2} + 1265.000T^{-1} + 103.574\times10^{-3}T$
1156-1800 K: $\Delta Hf° = -407.952 + 6.610\times10^{-3}T - 1.133\times10^{-6}T^{2} + 3312.900^{-}1$
$\Delta Gf° = -407.952 - 6.610\times10^{-3}T\ln T + 1.133\times10^{-6}T^{2} + 1656.450T^{-1} + 123.326\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Todd (497). Data from 298 to 398 K based on Todd (497), Hatta (202), and Volger (510). High-temperature data above 398 K based on Coughlin (103).

$Ba_2TiO_4(c)$
Barium Orthotitanate
[Formation: $2Ba(c,l) + Ti(c) + 2O_2(g) = Ba_2TiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°$_{298}$)/T	H°- H°$_{298}$	ΔHf°	ΔGf°	
298.15	35.800	47.000	47.000	0	-536.100	-509.813	373.698
300	35.890	47.220	47.000	.070	-536.091	-509.644	371.270
400	39.060	58.040	48.465	3.830	-535.819	-500.885	273.668
500	40.750	66.950	51.290	7.830	-535.740	-492.166	215.123
582	41.636	73.209	53.950	11.209	-536.060	-485.002	182.123
600	41.830	74.480	54.547	11.960	-536.014	-483.423	176.084
700	42.600	80.990	57.861	16.190	-535.859	-474.661	148.194
768	43.008	84.960	60.090	19.101	-535.876	-468.720	133.382
800	43.200	86.720	61.120	20.480	-535.890	-465.922	127.282
900	43.680	91.840	64.262	24.820	-535.874	-457.183	111.018
1000	44.070	96.460	67.250	29.210	-535.840	-448.436	98.004
1002	44.077	96.548	67.308	29.298	-535.841	-448.261	97.771
1002	44.077	96.548	67.308	29.298	-539.545	-448.261	97.771
1100	44.400	100.680	70.098	33.640	-539.615	-439.332	87.286
1156	44.551	102.884	71.632	36.127	-539.640	-434.222	82.092
1156	44.551	102.884	71.632	36.127	-540.657	-434.222	82.092
1200	44.670	104.550	72.808	38.090	-540.618	-430.171	78.344
1300	44.900	108.140	75.394	42.570	-540.513	-420.975	70.771
1400	45.080	111.470	77.849	47.070	-540.422	-411.780	64.281
1500	45.210	114.590	80.203	51.580	-540.352	-402.604	58.659
1600	45.310	117.510	82.441	56.110	-540.298	-393.418	53.738
1700	45.380	120.260	84.589	60.640	-540.278	-384.243	49.397
1800	45.400	122.850	86.639	65.180	-540.290	-375.057	45.538

Phase changes:
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K:
$Cp° = 42.623 + 1.908\times10^{-3}T - 6.571\times10^{5}T^{-2}$
$H° - H°_{298} = 42.623\times10^{-3}T + 0.954\times10^{-6}T^{2} + 6.571\times10^{2}T^{-1} - 14.997$

Formation equations (kcal/mol):

298.15-582 K:
$\Delta Hf° = -550.474 + 42.132\times10^{-3}T - 37.675\times10^{-6}T^{2} + 1538.900T^{-1}$
$\Delta Gf° = -550.474 - 42.132\times10^{-3}T\ln T + 37.675\times10^{-6}T^{2} + 769.450T^{-1} + 356.539\times10^{-3}T$

582-768 K:
$\Delta Hf° = -543.432 + 17.652\times10^{-3}T - 11.395\times10^{-6}T^{2} + 551.900T^{-1}$
$\Delta Gf° = -543.432 - 17.652\times10^{-3}T\ln T + 11.395\times10^{-6}T^{2} + 275.950T^{-1} + 205.341\times10^{-3}T$

768-1002 K:
$\Delta Hf° = -537.521 + 1.368\times10^{-3}T - 0.213\times10^{-6}T^{2} + 551.100T^{-1}$
$\Delta Gf° = -537.521 - 1.368\times10^{-3}T\ln T + 0.213\times10^{-6}T^{2} + 275.550T^{-1} + 98.045\times10^{-3}T$

1002-1156 K:
$\Delta Hf° = -552.029 + 9.502\times10^{-3}T - 2.473\times10^{-6}T^{2} + 5483.700T^{-1}$
$\Delta Gf° = -552.029 - 9.502\times10^{-3}T\ln T + 2.473\times10^{-6}T^{2} + 2741.850T^{-1} + 164.007\times10^{-3}T$

1156-1800 K:
$\Delta Hf° = -556.066 + 11.902\times10^{-3}T - 2.796\times10^{-6}T^{2} + 6266.600T^{-1}$
$\Delta Gf° = -556.066 - 11.902\times10^{-3}T\ln T + 2.796\times10^{-6}T^{2} + 3133.300T^{-1} + 183.759\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Todd (497). High-temperature data based on Coughlin (103).

$BaUO_4(c)$
Barium Uranate
[Formation: $Ba(c,l) + U(c) + 2O_2(g) = BaUO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	29.940	36.800	36.800	0	-477.320	-451.045	330.620
300	30.002	36.986	36.803	.055	-477.315	-450.881	328.462
400	32.818	46.054	38.017	3.215	-476.987	-442.120	241.560
500	34.348	53.554	40.400	6.577	-476.731	-433.438	189.453
582	35.188	58.837	42.631	9.432	-476.720	-426.340	160.095
600	35.373	59.912	43.134	10.067	-476.663	-424.783	154.725
700	36.164	65.425	45.932	13.645	-476.424	-416.155	129.928
768	36.614	68.800	47.808	16.122	-476.349	-410.306	116.759
800	36.826	70.299	48.678	17.297	-476.327	-407.555	111.337
900	37.416	74.673	51.330	21.009	-476.271	-398.964	96.880
942	37.645	76.385	52.409	22.585	-476.266	-395.357	91.724
942	37.645	76.385	52.409	22.585	-476.933	-395.357	91.724
1000	37.961	78.642	53.864	24.778	-476.863	-390.335	85.307
1002	37.976	78.718	53.914	24.854	-476.861	-390.162	85.099
1002	37.976	78.718	53.914	24.854	-478.713	-390.162	85.099
1049	38.331	80.467	55.064	26.647	-478.670	-386.009	80.420
1049	38.331	80.467	55.064	26.647	-479.807	-386.009	80.420
1100	38.717	82.285	56.286	28.599	-479.698	-381.451	75.786

Phase changes: 582 K, α − β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β − γ transition point of Ba; ΔH° = 0 kcal/mol.
942 K, α − β transition point of U; ΔH° = 0.667 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.
1049 K, β − γ transition point of U; ΔH° = 1.137 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp^\circ = 34.145 + 4.304\times10^{-3}T - 4.879\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 34.145\times10^{-3}T + 2.152\times10^{-6}T^2 + 4.879\times10^{2}T^{-1} - 12.008$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf^\circ = -486.547 + 26.298\times10^{-3}T - 21.326\times10^{-6}T^2 + 978.500T^{-1}$
$\Delta Gf^\circ = -486.547 - 26.298\times10^{-3}T\ln T + 21.326\times10^{-6}T^2 + 489.250T^{-1} + 257.048\times10^{-3}T$
582-768 K: $\Delta Hf^\circ = -483.026 + 14.058\times10^{-3}T - 8.186\times10^{-6}T^2 + 485.000T^{-1}$
$\Delta Gf^\circ = -483.026 - 14.058\times10^{-3}T\ln T + 8.186\times10^{-6}T^2 + 242.500T^{-1} + 181.449\times10^{-3}T$
768-942 K: $\Delta Hf^\circ = -480.070 + 5.916\times10^{-3}T - 2.595\times10^{-6}T^2 + 484.600T^{-1}$
$\Delta Gf^\circ = -480.070 - 5.916\times10^{-3}T\ln T + 2.595\times10^{-6}T^2 + 242.300T^{-1} + 127.801\times10^{-3}T$
942-1002 K: $\Delta Hf^\circ = -477.660 - 1.229\times10^{-3}T + 1.627\times10^{-6}T^2 + 397.100T^{-1}$
$\Delta Gf^\circ = -477.660 + 1.229\times10^{-3}T\ln T - 1.627\times10^{-6}T^2 + 198.550T^{-1} + 80.340\times10^{-3}T$
1002-1049 K: $\Delta Hf^\circ = -484.914 + 2.838\times10^{-3}T + 0.497\times10^{-6}T^2 + 2863.400T^{-1}$
$\Delta Gf^\circ = -484.914 - 2.838\times10^{-3}T\ln T - 0.497\times10^{-6}T^2 + 1431.700T^{-1} + 113.321\times10^{-3}T$
1049-1100 K: $\Delta Hf^\circ = -487.210 + 3.943\times10^{-3}T + 0.497\times10^{-6}T^2 + 2863.400T^{-1}$
$\Delta Gf^\circ = -487.210 - 3.943\times10^{-3}T\ln T - 0.497\times10^{-6}T^2 + 1431.700T^{-1} + 123.196\times10^{-3}T$

Source: Data from O'Hare (367).

$BaZrO_3$(c)
Barium Zirconate
[Formation: Ba(c,l) + Zr(c) + $1.5O_2$(g) = $BaZrO_3$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.310	29.830	29.830	0	-425.300	-405.051	296.907
300	24.357	29.981	29.831	.045	-425.297	-404.924	294.983
400	26.320	37.292	30.815	2.591	-425.182	-398.154	217.539
500	27.552	43.305	32.729	5.288	-425.157	-391.403	171.080
582	28.347	47.550	34.524	7.581	-425.317	-385.857	144.893
600	28.522	48.416	34.928	8.093	-425.292	-384.637	140.102
700	29.369	52.878	37.181	10.988	-425.191	-377.871	117.975
760	29.844	55.313	38.517	12.765	-425.170	-373.818	107.496
760	27.810	55.313	38.517	12.765	-425.170	-373.818	107.496
768	27.802	55.604	38.693	12.987	-425.183	-373.277	106.222
800	27.772	56.738	39.393	13.876	-425.241	-371.113	101.382
900	27.678	60.004	41.505	16.649	-425.423	-364.335	88.472
1000	27.584	62.915	43.503	19.412	-425.647	-357.537	78.139
1002	27.582	62.970	43.542	19.467	-425.653	-357.401	77.953
1002	27.582	62.970	43.542	19.467	-427.505	-357.401	77.953
1100	27.489	65.540	45.389	22.166	-427.818	-350.528	69.643
1136	27.455	66.425	46.042	23.155	-427.936	-347.997	66.949
1136	27.455	66.425	46.042	23.155	-428.887	-347.997	66.949
1175	27.418	67.351	46.734	24.225	-428.961	-345.218	64.210
1175	30.840	67.606	46.734	24.525	-428.661	-345.218	64.210
1200	30.840	68.255	47.175	25.296	-428.624	-343.443	62.549
1300	30.840	70.724	48.893	28.380	-428.481	-336.351	56.545
1400	30.840	73.009	50.535	31.464	-428.366	-329.269	51.400
1500	30.840	75.137	52.105	34.548	-428.275	-322.193	46.943
1600	30.840	77.127	53.607	37.632	-428.212	-315.123	43.043

Phase changes:
582 K, α - β transition point of Ba; $\Delta H^\circ = 0$ kcal/mol.
760 K, α - β transition point of $BaZrO_3$ $\Delta H^\circ = 0$ kcal/mol.
768 K, β - γ transition point of Ba; $\Delta H^\circ = 0$ kcal/mol.
1002 K, melting point of Ba; $\Delta H^\circ = 1.852$ kcal/mol.
1136 K, α - β transition point of Zr; $\Delta H^\circ = 0.951$ kcal/mol.
1175 K, β - γ transition point of $BaZrO_3$ $\Delta H^\circ = 0.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-760 K: $Cp^\circ = 25.273 + 6.594\times10^{-3}T - 2.545\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 25.273\times10^{-3}T + 3.297\times10^{-6}T^2 + 2.545\times10^{2}T^{-1} - 8.682$
760-1175 K: $Cp^\circ = 28.528 - 0.944\times10^{-3}T$
$H^\circ - H^\circ_{298} = 28.528\times10^{-3}T - 0.472\times10^{-6}T^2 - 8.644$
1175-1600 K: $Cp^\circ = 30.840$
$H^\circ - H^\circ_{298} = 30.840\times10^{-3}T - 11.712$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf^\circ = -431.405 + 18.158\times10^{-3}T - 16.649\times10^{-6}T^2 + 647.300T^{-1}$
$\Delta Gf^\circ = -431.405 - 18.158\times10^{-3}T\ln T + 16.649\times10^{-6}T^2 + 323.650T^{-1} + 183.243\times10^{-3}T$
582-760 K: $\Delta Hf^\circ = -427.884 + 5.918\times10^{-3}T - 3.509\times10^{-6}T^2 + 153.800T^{-1}$
$\Delta Gf^\circ = -427.884 - 5.918\times10^{-3}T\ln T + 3.509\times10^{-6}T^2 + 76.900T^{-1} + 107.644\times10^{-3}T$
760-768 K: $\Delta Hf^\circ = -427.846 + 9.173\times10^{-3}T - 7.278\times10^{-6}T^2 - 100.700T^{-1}$
$\Delta Gf^\circ = -427.846 - 9.173\times10^{-3}T\ln T + 7.278\times10^{-6}T^2 - 50.350T^{-1} + 126.541\times10^{-3}T$
768-1002 K: $\Delta Hf^\circ = -424.890 + 1.031\times10^{-3}T - 1.688\times10^{-6}T^2 - 101.100T^{-1}$
$\Delta Gf^\circ = -424.890 - 1.031\times10^{-3}T\ln T + 1.688\times10^{-6}T^2 - 50.550T^{-1} + 72.893\times10^{-3}T$
1002-1136 K: $\Delta Hf^\circ = -432.144 + 5.098\times10^{-3}T - 2.817\times10^{-6}T^2 + 2365.200T^{-1}$
$\Delta Gf^\circ = -432.144 - 5.098\times10^{-3}T\ln T + 2.817\times10^{-6}T^2 + 1182.600T^{-1} + 105.874\times10^{-3}T$
1136-1175 K: $\Delta Hf^\circ = -434.640 + 6.267\times10^{-3}T - 2.687\times10^{-6}T^2 + 2419.700T^{-1}$
$\Delta Gf^\circ = -434.640 - 6.267\times10^{-3}T\ln T + 2.687\times10^{-6}T^2 + 1209.850T^{-1} + 116.423\times10^{-3}T$
1175-1600 K: $\Delta Hf^\circ = -437.708 + 8.579\times10^{-3}T - 2.214\times10^{-6}T^2 + 2419.700T^{-1}$
$\Delta Gf^\circ = -437.708 - 8.579\times10^{-3}T\ln T + 2.214\times10^{-6}T^2 + 1209.850T^{-1} + 135.933\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from King (270). High-temperature data based on Levitskii (307).

$BeAl_2O_4$(c,l)
Beryllium Aluminate, Chrysoberyl
[Formation: $Be(c,l) + 2Al(c,l) + 2O_2(g) = BeAl_2O_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	25.182	15.845	15.845	0	-549.900	-520.685	381.668
300	25.320	16.001	15.845	.047	-549.908	-520.505	379.183
400	31.138	24.152	16.917	2.894	-550.113	-510.662	279.009
500	34.716	31.515	19.115	6.200	-550.018	-500.808	218.900
600	37.039	38.064	21.739	9.795	-549.780	-490.980	178.837
700	38.659	43.901	24.494	13.585	-549.485	-481.205	150.237
800	39.873	49.147	27.254	17.514	-549.188	-471.474	128.799
900	40.839	53.901	29.955	21.551	-548.916	-461.774	112.132
933.61	41.107	55.403	30.845	22.928	-548.835	-458.521	107.334
933.61	41.107	55.403	30.845	22.928	-553.995	-458.521	107.334
1000	41.635	58.246	32.572	25.674	-553.785	-451.743	98.727
1100	42.311	62.247	35.090	29.873	-553.444	-441.555	87.728
1200	42.897	65.954	37.508	34.135	-553.079	-431.401	78.568
1300	43.420	69.407	39.829	38.451	-552.699	-421.270	70.821
1400	43.917	72.643	42.059	42.818	-552.306	-411.173	64.186
1500	44.434	75.691	44.201	47.235	-551.896	-401.121	58.442
1527	44.595	76.485	44.765	48.437	-551.782	-398.402	57.020
1527	44.595	76.485	44.765	48.437	-552.393	-398.402	57.020
1560	44.792	77.441	45.447	49.911	-552.254	-395.084	55.349
1560	44.792	77.441	45.447	49.911	-555.173	-395.084	55.349
1600	45.031	78.578	46.261	51.707	-554.968	-390.981	53.405
1700	45.784	81.329	48.244	56.245	-554.416	-380.759	48.949
1800	46.795	83.972	50.154	60.872	-553.787	-370.561	44.992
1900	48.176	86.539	52.004	65.617	-553.052	-360.386	41.453
2000	50.069	89.056	53.794	70.523	-552.166	-350.274	38.276
2100	52.627	91.556	55.531	75.652	-551.069	-340.208	35.405
2146	54.075	92.713	56.315	78.110	-550.469	-335.594	34.177
2146	50.340	111.800	56.315	119.070	-509.509	-335.594	34.177
2200	54.390	113.101	57.692	121.900	-508.863	-331.220	32.903
2300	61.880	115.684	60.154	127.720	-507.097	-323.180	30.709
2400	69.380	118.476	62.526	134.280	-504.601	-315.236	28.706
2500	76.870	121.460	64.824	141.590	-501.365	-307.405	26.873

Phase changes:
933.61 K, melting point of Al; $\Delta H^\circ = 2.580$ kcal/mol.
1527 K, $\alpha - \beta$ transition point of Be; $\Delta H^\circ = 0.611$ kcal/mol.
1560 K, melting point of Be; $\Delta H^\circ = 2.919$ kcal/mol.
2146 K, melting point of $BeAl_2O_4$; $\Delta H^\circ = 40.960$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2146 K: $Cp^\circ = 35.589 + 6.884\times10^{-3}T - 11.076\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 35.589\times10^{-3}T + 3.442\times10^{-6}T^2 + 11.076\times10^{2}T^{-1} - 14.632$
2146-2500 K: $Cp^\circ = -110.500 + 74.956\times10^{-3}T$
$H^\circ - H^\circ_{298} = -110.500\times10^{-3}T + 37.478\times10^{-6}T^2 + 183.605$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -554.987 + 7.204\times10^{-3}T - 1.980\times10^{-6}T^2 + 928.900T^{-1}$
$\Delta Gf^\circ = -554.987 - 7.204\times10^{-3}T\ln T + 1.980\times10^{-6}T^2 + 464.450T^{-1} + 150.281\times10^{-3}T$
933.61-1527 K: $\Delta Hf^\circ = -557.523 + 1.208\times10^{-3}T + 1.474\times10^{-6}T^2 + 894.100T^{-1}$
$\Delta Gf^\circ = -557.523 - 1.208\times10^{-3}T\ln T - 1.474\times10^{-6}T^2 + 447.050T^{-1} + 115.234\times10^{-3}T$
1527-1560 K: $\Delta Hf^\circ = -555.939 - 1.751\times10^{-3}T + 2.436\times10^{-6}T^2 + 1017.200T^{-1}$
$\Delta Gf^\circ = -555.939 + 1.751\times10^{-3}T\ln T - 2.436\times10^{-6}T^2 + 508.600T^{-1} + 93.947\times10^{-3}T$
1560-2000 K: $\Delta Hf^\circ = -559.888 - 1.091\times10^{-3}T + 2.436\times10^{-6}T^2 + 1017.200T^{-1}$
$\Delta Gf^\circ = -559.888 + 1.091\times10^{-3}T\ln T - 2.436\times10^{-6}T^2 + 508.600T^{-1} + 101.331\times10^{-3}T$
2000-2146 K: $\Delta Hf^\circ = -557.215 - 3.311\times10^{-3}T + 3.024\times10^{-6}T^2 - 152.400T^{-1}$
$\Delta Gf^\circ = -557.215 + 3.311\times10^{-3}T\ln T - 3.024\times10^{-6}T^2 - 76.200T^{-1} + 84.443\times10^{-3}T$
2146-2500 K: $\Delta Hf^\circ = -358.979 - 149.400\times10^{-3}T + 37.060\times10^{-6}T^2 - 1260.000T^{-1}$
$\Delta Gf^\circ = -358.979 + 149.400\times10^{-3}T\ln T - 37.060\times10^{-6}T^2 - 630.000T^{-1} - 1055.472\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Furukawa (167). High-temperature data based on Ditmars (123) and Ishihara (215).

$BeAl_6O_{10}(c)$
Beryllium Trialuminate
[Formation: $Be(c,l) + 6Al(c,l) + 5O_2(g) = BeAl_6O_{10}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	63.381	41.958	41.958	0	-1344.900	-1271.557	932.065
300	63.706	42.351	41.958	.118	-1344.920	-1271.103	925.986
400	77.502	62.734	44.644	7.236	-1345.376	-1246.402	680.993
500	85.690	80.984	50.124	15.430	-1345.082	-1221.681	533.989
600	90.956	97.104	56.639	24.279	-1344.459	-1197.044	436.018
700	94.666	111.420	63.463	33.570	-1343.725	-1172.536	366.078
800	97.473	124.250	70.271	43.183	-1343.014	-1148.134	313.652
900	99.725	135.870	76.930	53.046	-1342.398	-1123.816	272.896
933.61	100.362	139.538	79.118	56.408	-1342.221	-1115.656	261.162
933.61	100.362	139.538	79.118	56.408	-1357.701	-1115.656	261.162
1000	101.620	146.470	83.354	63.116	-1357.201	-1098.457	240.065
1100	103.270	156.240	89.547	73.362	-1356.366	-1072.630	213.109
1200	104.740	165.290	95.487	83.763	-1355.442	-1046.877	190.660
1300	106.100	173.720	101.176	94.307	-1354.438	-1021.189	171.675
1400	107.370	181.630	106.644	104.981	-1353.366	-995.592	155.417
1500	108.570	189.080	111.895	115.778	-1352.222	-970.096	141.341
1527	108.881	191.020	113.277	118.714	-1351.902	-963.214	137.857
1527	108.881	191.020	113.277	118.714	-1352.513	-963.214	137.857
1560	109.260	193.358	114.952	122.313	-1352.118	-954.821	133.765
1560	109.260	193.358	114.952	122.313	-1355.037	-954.821	133.765
1600	109.720	196.130	116.947	126.693	-1354.518	-944.564	129.020
1700	110.820	202.810	121.798	137.721	-1353.158	-918.985	118.142
1800	111.900	209.180	126.482	148.857	-1351.720	-893.494	108.484
1900	112.950	215.260	130.997	160.099	-1350.206	-868.060	99.848
2000	113.980	221.080	135.357	171.446	-1348.612	-842.732	92.088
2100	114.990	226.660	139.568	182.894	-1346.947	-817.474	85.075
2150	115.490	229.370	141.623	188.656	-1346.085	-804.873	81.815

Phase changes: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2150 K: $Cp° = 90.902 + 12.698\times10^{-3}T - 27.830\times10^{5}T^{-2}$
$H°- H°_{298} = 90.902\times10^{-3}T + 6.349\times10^{-6}T^{2} + 27.830\times10^{2}T^{-1} - 37.001$

Formation equations (kcal/mol):

298.15- 933.61 K: $\Delta Hf° = -1359.444 + 22.459\times10^{-3}T - 7.490\times10^{-6}T^{2} + 2538.300T^{-1}$
$\Delta Gf° = -1359.444 - 22.459\times10^{-3}T\ln T + 7.490\times10^{-6}T^{2} + 1269.150T^{-1} + 406.225\times10^{-3}T$
933.61-1527 K: $\Delta Hf° = -1367.050 + 4.471\times10^{-3}T + 2.872\times10^{-6}T^{2} + 2433.900T^{-1}$
$\Delta Gf° = -1367.050 - 4.471\times10^{-3}T\ln T - 2.872\times10^{-6}T^{2} + 1216.950T^{-1} + 301.086\times10^{-3}T$
1527-1560 K: $\Delta Hf° = -1365.466 + 1.512\times10^{-3}T + 3.834\times10^{-6}T^{2} + 2557.000T^{-1}$
$\Delta Gf° = -1365.466 - 1.512\times10^{-3}T\ln T - 3.834\times10^{-6}T^{2} + 1278.500T^{-1} + 279.798\times10^{-3}T$
1560-2000 K: $\Delta Hf° = -1369.415 + 2.172\times10^{-3}T + 3.834\times10^{-6}T^{2} + 2557.000T^{-1}$
$\Delta Gf° = -1369.415 - 2.172\times10^{-3}T\ln T - 3.834\times10^{-6}T^{2} + 1278.500T^{-1} + 287.182\times10^{-3}T$
2000-2150 K: $\Delta Hf° = -1362.733 - 3.378\times10^{-3}T + 5.304\times10^{-6}T^{2} - 367.000T^{-1}$
$\Delta Gf° = -1362.733 + 3.378\times10^{-3}T\ln T - 5.304\times10^{-6}T^{2} - 183.500T^{-1} + 244.962\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Furukawa (168). High-temperature data from Ditmars (124).

$BeBO_2(g)$
Beryllium Boron Dioxide (ideal gas)
[Formation: $Be(c,l) + B(\beta) + O_2(g) = BeBO_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.990	63.404	63.404	0	-115.200	-118.396	86.785
300	12.027	63.478	63.405	.022	-115.203	-118.416	86.265
400	13.741	67.185	63.897	1.315	-115.373	-119.463	65.271
500	15.009	70.394	64.884	2.755	-115.572	-120.463	52.654
600	15.951	73.218	66.041	4.306	-115.796	-121.419	44.226
700	16.663	75.733	67.250	5.938	-116.035	-122.340	38.196
800	17.212	77.995	68.454	7.633	-116.282	-123.222	33.662
900	17.641	80.048	69.630	9.376	-116.539	-124.071	30.128
1000	17.980	81.925	70.767	11.158	-116.810	-124.895	27.295
1100	18.251	83.652	71.861	12.970	-117.103	-125.696	24.973
1200	18.471	85.250	72.911	14.807	-117.416	-126.466	23.032
1300	18.650	86.736	73.918	16.663	-117.756	-127.198	21.384
1400	18.799	88.123	74.883	18.536	-118.123	-127.909	19.967
1500	18.922	89.425	75.810	20.422	-118.519	-128.602	18.737
1527	18.950	89.763	76.054	20.933	-118.631	-128.777	18.431
1527	18.950	89.763	76.054	20.933	-119.242	-128.777	18.431
1560	18.985	90.168	76.348	21.559	-119.384	-129.001	18.072
1560	18.985	90.168	76.348	21.559	-122.303	-129.001	18.072
1600	19.027	90.649	76.700	22.319	-122.449	-129.169	17.643
1700	19.115	91.806	77.555	24.227	-122.819	-129.588	16.660
1800	19.191	92.900	78.377	26.142	-123.202	-129.966	15.780
1900	19.256	93.940	79.169	28.064	-123.598	-130.315	14.989
2000	19.312	94.929	79.933	29.993	-124.006	-130.672	14.279

*Data estimated.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 15.485 + 2.500\times10^{-3}T - 3.770\times10^{5}T^{-2}$
$H°-H°_{298} = 15.485\times10^{-3}T + 1.250\times10^{-6}T^{2} + 3.770\times10^{2}T^{-1} - 5.992$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = -114.716 - 1.209\times10^{-3}T - 0.907\times10^{-6}T^{2} - 12.800T^{-1}$
$\Delta Gf° = -114.716 + 1.209\times10^{-3}T\ln T + 0.907\times10^{-6}T^{2} - 6.400T^{-1} - 19.429\times10^{-3}T$
1527-1560 K: $\Delta Hf° = -113.132 - 4.168\times10^{-3}T + 0.055\times10^{-6}T^{2} + 110.300T^{-1}$
$\Delta Gf° = -113.132 + 4.168\times10^{-3}T\ln T - 0.055\times10^{-6}T^{2} + 55.150T^{-1} - 40.716\times10^{-3}T$
1560-2000 K: $\Delta Hf° = -117.081 - 3.508\times10^{-3}T + 0.055\times10^{-6}T^{2} + 110.300T^{-1}$
$\Delta Gf° = -117.081 + 3.508\times10^{-3}T\ln T - 0.055\times10^{-6}T^{2} + 55.150T^{-1} - 33.333\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$BeB_2O_4(g)$
Beryllium Diborate (ideal gas)
[Formation: $Be(c,l) + 2B(\beta) + 2O_2(g) = BeB_2O_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	21.932	78.079	78.079	0	-323.000	-315.540	231.294
300	22.001	78.215	78.079	.041	-323.002	-315.492	229.833
400	25.297	85.016	78.986	2.412	-323.121	-312.975	171.000
500	27.839	90.946	80.796	5.075	-323.235	-310.422	135.684
600	29.782	96.202	82.935	7.960	-323.355	-307.850	112.133
700	31.266	100.909	85.172	11.016	-323.466	-305.257	95.304
800	32.407	105.162	87.410	14.202	-323.566	-302.648	82.678
900	33.294	109.032	89.600	17.489	-323.662	-300.023	72.854
1000	33.989	112.577	91.723	20.854	-323.765	-297.392	64.994
1100	34.543	115.844	93.769	24.282	-323.885	-294.761	58.563
1200	34.988	118.869	95.737	27.759	-324.025	-292.109	53.200
1300	35.350	121.685	97.626	31.277	-324.193	-289.430	48.657
1400	35.647	124.315	99.439	34.827	-324.395	-286.748	44.763
1500	35.895	126.784	101.181	38.405	-324.632	-284.054	41.386
1527	35.951	127.425	101.639	39.375	-324.704	-283.317	40.549
1527	35.951	127.425	101.639	39.375	-325.315	-283.317	40.549
1560	36.019	128.194	102.192	40.563	-325.407	-282.439	39.568
1560	36.019	128.194	102.192	40.563	-328.326	-282.439	39.568
1600	36.102	129.107	102.854	42.005	-328.414	-281.260	38.418
1700	36.278	131.301	104.463	45.624	-328.647	-278.315	35.779
1800	36.427	133.379	106.013	49.259	-328.904	-275.327	33.429
1900	36.555	135.352	107.505	52.909	-329.186	-272.323	31.324
2000	36.666	137.230	108.945	56.570	-329.495	-269.351	29.433

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 29.151 + 4.844\times10^{-3}T - 7.702\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 29.151\times10^{-3}T + 2.422\times10^{-6}T^{2} + 7.702\times10^{2}T^{-1} - 11.490$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf^\circ = -323.449 + 0.504\times10^{-3}T - 0.930\times10^{-6}T^{2} + 113.700T^{-1}$
$\Delta Gf^\circ = -323.449 - 0.504\times10^{-3}T\ln T + 0.930\times10^{-6}T^{2} + 56.850T^{-1} + 28.482\times10^{-3}T$
1527-1560 K: $\Delta Hf^\circ = -321.865 - 2.455\times10^{-3}T + 0.032\times10^{-6}T^{2} + 236.800T^{-1}$
$\Delta Gf^\circ = -321.865 + 2.455\times10^{-3}T\ln T - 0.032\times10^{-6}T^{2} + 118.400T^{-1} + 7.194\times10^{-3}T$
1560-2000 K: $\Delta Hf^\circ = -325.814 - 1.795\times10^{-3}T + 0.032\times10^{-6}T^{2} + 236.800T^{-1}$
$\Delta Gf^\circ = -325.814 + 1.795\times10^{-3}T\ln T - 0.032\times10^{-6}T^{2} + 118.400T^{-1} + 14.578\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$Be_3B_2O_6(c)$
Triberyllium Diborate
[Formation: $3Be(c,l) + 2B(\beta) + 3O_2(g) = Be_3B_2O_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	33.400	24.000	24.000	0	-741.960	-702.412	514.875
300	33.560	24.207	24.000	.062	-741.968	-702.167	511.522
400	41.830	35.033	25.421	3.845	-742.257	-688.850	376.365
500	48.480	45.100	28.362	8.369	-742.243	-675.496	295.255
600	54.160	54.451	31.941	13.506	-741.956	-662.162	241.189
700	59.170	63.187	35.787	19.180	-741.377	-648.913	202.597
800	63.290	71.369	39.729	25.312	-740.525	-635.756	173.678
900	66.340	79.009	43.673	31.802	-739.466	-622.711	151.213
1000	68.420	86.112	47.567	38.545	-738.294	-609.806	133.271
1100	69.840	92.703	51.374	45.462	-737.088	-597.028	118.617
1200	70.840	98.825	55.077	52.498	-735.883	-584.360	106.425
1300	71.600	104.526	58.664	59.621	-734.714	-571.755	96.120
1400	72.230	109.856	62.132	66.813	-733.594	-559.262	87.304
1500	72.790	114.858	65.482	74.064	-732.526	-546.870	79.678
1527	72.930	116.158	66.367	76.031	-732.248	-543.513	77.789
1527	72.930	116.158	66.367	76.031	-734.081	-543.513	77.789
1560	73.102	117.720	67.437	78.441	-733.750	-539.447	75.573
1560	73.102	117.720	67.437	78.441	-742.507	-539.447	75.573
1600	73.310	119.573	68.717	81.369	-742.024	-534.242	72.973
1700	73.830	124.032	71.840	88.726	-740.809	-521.322	67.020
1800	74.380	128.268	74.859	96.137	-739.586	-508.434	61.731

*Data except enthalpy of formation at 298 K and temperature of fusion estimated.

Phase changes: 1527 K, α − β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 48.156 + 19.134\times10^{-3}T - 18.188\times10^{5}T^{-2}$
$H° - H°_{298} = 48.156\times10^{-3}T + 9.567\times10^{-6}T^{2} + 18.188\times10^{2}T^{-1} - 21.308$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = -746.052 + 2.797\times10^{-3}T + 3.788\times10^{-6}T^{2} + 870.900T^{-1}$
$\Delta Gf° = -746.052 - 2.797\times10^{-3}T\ln T - 3.788\times10^{-6}T^{2} + 435.450T^{-1} + 158.535\times10^{-3}T$
1527-1560 K: $\Delta Hf° = -741.301 - 6.080\times10^{-3}T + 6.674\times10^{-6}T^{2} + 1240.200T^{-1}$
$\Delta Gf° = -741.301 + 6.080\times10^{-3}T\ln T - 6.674\times10^{-6}T^{2} + 620.100T^{-1} + 94.674\times10^{-3}T$
1560-1800 K: $\Delta Hf° = -753.147 - 4.100\times10^{-3}T + 6.674\times10^{-6}T^{2} + 1240.200T^{-1}$
$\Delta Gf° = -753.147 + 4.100\times10^{-3}T\ln T - 6.674\times10^{-6}T^{2} + 620.100T^{-1} + 116.825\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K and temperature of fusion.

Be_2C(c,l)
Diberyllium Carbide
[Formation: $2Be(c,l) + C(c) = Be_2C(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.340	4.000	4.000	0	-28.000	-27.430	20.106
300	10.350	4.064	4.001	.019	-27.999	-27.429	19.982
400	10.860	7.111	4.411	1.080	-28.054	-27.233	14.879
500	11.371	9.590	5.208	2.191	-28.262	-27.014	11.807
600	11.882	11.708	6.118	3.354	-28.566	-26.726	9.735
700	12.392	13.578	7.052	4.568	-28.926	-26.400	8.242
800	12.903	15.266	7.976	5.832	-29.317	-26.011	7.106
900	13.413	16.815	8.873	7.148	-29.722	-25.568	6.209
1000	13.924	18.255	9.740	8.515	-30.138	-25.088	5.483
1100	14.435	19.606	10.576	9.933	-30.568	-24.553	4.878
1200	14.945	20.884	11.382	11.402	-31.003	-24.008	4.372
1300*	15.456	22.100	12.160	12.922	-31.445	-23.394	3.933
1400	15.966	23.264	12.912	14.493	-31.889	-22.757	3.552
1500	16.477	24.383	13.640	16.115	-32.333	-22.109	3.221
1527	16.615	24.678	13.832	16.562	-32.453	-21.912	3.136
1527	16.615	24.678	13.832	16.562	-33.675	-21.912	3.136
1560	16.784	25.035	14.065	17.114	-33.820	-21.672	3.036
1560	16.784	25.035	14.065	17.114	-39.658	-21.672	3.036
1600	16.988	25.463	14.345	17.789	-39.777	-21.206	2.897
1700	17.498	26.508	15.030	19.513	-40.043	-20.061	2.579
1800	18.009	27.523	15.696	21.288	-40.263	-18.888	2.293
1900	18.519	28.510	16.344	23.115	-40.436	-17.659	2.031
2000	19.030	29.473	16.977	24.992	-40.565	-16.461	1.799
2100	19.541	30.414	17.594	26.921	-40.646	-15.270	1.589
2200	20.051	31.335	18.199	28.900	-40.681	-14.050	1.396
2300	20.562	32.237	18.789	30.931	-40.668	-12.850	1.221
2400	21.072	33.123	19.368	33.012	-40.610	-11.642	1.060
2400	21.072	40.623	19.368	51.012	-22.610	-11.642	1.060
2500	21.072	41.483	20.235	53.119	-22.528	-11.173	.977
2600	21.072	42.310	21.069	55.226	-22.451	-10.754	.904
2700	21.072	43.105	21.871	57.333	-22.377	-10.281	.832

*Data estimated above 1200 K.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.
2400 K, melting point of Be_2C; ΔH° = 18.000 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2400 K: $Cp° = 8.818 + 5.106\times10^{-3}T$
$H°-H°_{298} = 8.818\times10^{-3}T + 2.553\times10^{-6}T^2 - 2.856$
2400-3000 K: $Cp° = 21.072$
$H°-H°_{298} = 21.072\times10^{-3}T + 0.439$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = -25.337 - 4.182\times10^{-3}T - 0.137\times10^{-6}T^2 - 418.500T^{-1}$
$\Delta Gf° = -25.337 + 4.182\times10^{-3}T\ln T + 0.137\times10^{-6}T^2 - 209.250T^{-1} - 28.533\times10^{-3}T$
1527-1560 K: $\Delta Hf° = -22.170 - 10.100\times10^{-3}T + 1.787\times10^{-6}T^2 - 172.300T^{-1}$
$\Delta Gf° = -22.170 + 10.100\times10^{-3}T\ln T - 1.787\times10^{-6}T^2 - 86.150T^{-1} - 71.107\times10^{-3}T$
1560-2000 K: $\Delta Hf° = -30.067 - 8.780\times10^{-3}T + 1.787\times10^{-6}T^2 - 172.300T^{-1}$
$\Delta Gf° = -30.067 + 8.780\times10^{-3}T\ln T - 1.787\times10^{-6}T^2 - 86.150T^{-1} - 56.340\times10^{-3}T$
2000-2400 K: $\Delta Hf° = -28.075 - 10.903\times10^{-3}T + 2.419\times10^{-6}T^2 - 720.000T^{-1}$
$\Delta Gf° = -28.075 + 10.903\times10^{-3}T\ln T - 2.419\times10^{-6}T^2 - 360.000T^{-1} - 72.140\times10^{-3}T$
2400-2745 K: $\Delta Hf° = -24.780 + 1.351\times10^{-3}T - 0.134\times10^{-6}T^2 - 720.000T^{-1}$
$\Delta Gf° = -24.780 - 1.351\times10^{-3}T\ln T + 0.134\times10^{-6}T^2 - 360.000T^{-1} + 15.735\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Other data from Schick (437) who estimated heat capacities above 1200 K.

$BeCO_3(c)$
Beryllium Carbonate
[Formation: $Be(c) + C(c) + 1.5O_2(g) = BeCO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.530	12.430	12.430	0	-250.000	-230.704	169.108
300	15.650	12.520	12.430	.030	-250.001	-230.582	167.977
400	20.140	17.720	13.120	1.840	-249.936	-224.120	122.452
500	22.720	22.510	14.510	4.000	-249.690	-217.686	95.149
600	24.550	26.820	16.220	6.360	-249.385	-211.315	76.970
700	26.010	30.720	18.020	8.890	-249.021	-205.005	64.004
800	27.290	34.280	19.830	11.560	-248.605	-198.741	54.293
900	28.460	37.560	21.616	14.350	-248.139	-192.529	46.752
1000	29.560	40.610	23.360	17.250	-247.625	-186.375	40.732

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 20.883 + 9.462 \times 10^{-3}T - 7.266 \times 10^{5}T^{-2}$
$H°- H°_{298} = 20.883 \times 10^{-3}T + 4.731 \times 10^{-6}T^{2} + 7.266 \times 10^{2}T^{-1} - 9.084$

Formation equations (kcal/mol):

298.15-1000 K: $ΔHf° = -251.949 + 1.779 \times 10^{-3}T + 2.248 \times 10^{-6}T^{2} + 363.400T^{-1}$
$ΔGf° = -251.949 - 1.779 \times 10^{-3}T\ln T - 2.248 \times 10^{-6}T^{2} + 181.700T^{-1} + 80.019 \times 10^{-3}T$

Source: Data are those estimated by Gurvich (196).

BeH(g)
Beryllium Hydride (ideal gas)
[Formation: Be(c,l) + $0.5H_2(g)$ = BeH(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	6.985	42.234	42.234	0	82.995	75.732	-55.512
300	6.986	42.277	42.234	.013	82.995	75.686	-55.136
400	7.060	44.295	42.510	.714	82.912	73.260	-40.027
500	7.205	45.885	43.031	1.427	82.775	70.859	-30.972
600	7.395	47.215	43.620	2.157	82.610	68.496	-24.949
700	7.597	48.370	44.217	2.907	82.434	66.153	-20.654
800	7.791	49.397	44.802	3.676	82.252	63.841	-17.440
900	7.967	50.325	45.365	4.464	82.067	61.554	-14.947
1000	8.124	51.173	45.904	5.269	81.876	59.283	-12.956
1100	8.262	51.954	46.419	6.088	81.670	57.032	-11.331
1200	8.383	52.678	46.911	6.921	81.451	54.798	-9.980
1300	8.490	53.353	47.381	7.764	81.215	52.592	-8.841
1400	8.585	53.986	47.830	8.618	80.964	50.400	-7.868
1500	8.670	54.581	48.260	9.481	80.694	48.217	-7.025
1527	8.691	54.736	48.373	9.715	80.618	47.639	-6.818
1527	8.691	54.736	48.373	9.715	80.007	47.639	-6.818
1560	8.717	54.922	48.510	10.003	79.912	46.932	-6.575
1560	8.717	54.922	48.510	10.003	76.993	46.932	-6.575
1600	8.748	55.143	48.673	10.352	76.905	46.164	-6.306
1700	8.818	55.676	49.070	11.230	76.685	44.237	-5.687
1800	8.884	56.182	49.451	12.115	76.467	42.330	-5.139
1900	8.944	56.664	49.818	13.007	76.253	40.457	-4.654
2000	8.999	57.124	50.172	13.904	76.038	38.577	-4.215

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 6.627 + 1.380\times10^{-3}T - 0.048\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 6.627\times10^{-3}T + 0.690\times10^{-6}T^{2} + 0.048\times10^{2}T^{-1} - 2.053$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf^\circ = 83.807 - 1.342\times10^{-3}T - 0.481\times10^{-6}T^{2} - 110.050T^{-1}$
$\Delta Gf^\circ = 83.807 + 1.342\times10^{-3}T\ln T + 0.481\times10^{-6}T^{2} - 55.025T^{-1} - 34.255\times10^{-3}T$
1527-1560 K: $\Delta Hf^\circ = 85.391 - 4.301\times10^{-3}T + 0.481\times10^{-6}T^{2} + 13.050T^{-1}$
$\Delta Gf^\circ = 85.391 + 4.301\times10^{-3}T\ln T - 0.481\times10^{-6}T^{2} + 6.525T^{-1} - 55.542\times10^{-3}T$
1560-2000 K: $\Delta Hf^\circ = 81.442 - 3.641\times10^{-3}T + 0.481\times10^{-6}T^{2} + 13.050T^{-1}$
$\Delta Gf^\circ = 81.442 + 3.641\times10^{-3}T\ln T - 0.481\times10^{-6}T^{2} + 6.525T^{-1} - 48.158\times10^{-3}T$

Source: Data from Gurvich (196).

BeH_2(amorphous)
Beryllium Dihydride
[Formation: $Be(c) + H_2(g) = BeH_2(amorphous)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.134	5.760	5.760	0	-4.540	3.724	-2.730
300	7.160	5.804	5.761	.013	-4.547	3.774	-2.749
400	8.588	8.060	6.058	.801	-4.889	6.602	-3.607
500	10.016	10.130	6.668	1.731	-5.159	9.504	-4.154

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp° = 3.007 + 14.044 \times 10^{-3}T - 0.053 \times 10^{5}T^{-2}$

$H°-H°_{298} = 3.007 \times 10^{-3}T + 7.022 \times 10^{-6}T^{2} + 0.053 \times 10^{2}T^{-1} - 1.539$

Formation equations (kcal/mol):

298.15-500 K: $\Delta Hf° = -2.260 - 8.190 \times 10^{-3}T + 5.641 \times 10^{-6}T^{2} - 101.300T^{-1}$

$\Delta Gf° = -2.260 + 8.190 \times 10^{-3}T\ln T - 5.641 \times 10^{-6}T^{2} - 50.650T^{-1} - 24.342 \times 10^{-3}T$

Source: Data from Gurvich (196).

$BeH_2(g)$
Beryllium Dihydride (ideal gas)
[Formation: $Be(c,l) + H_2(g) = BeH_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.259	41.350	41.350	0	30.000	27.653	-20.270
300	7.268	41.395	41.352	.013	29.993	27.637	-20.133
400	7.943	43.571	41.643	.771	29.621	26.907	-14.701
500	8.805	45.435	42.219	1.608	29.258	26.268	-11.482
600	9.667	47.117	42.897	2.532	28.937	25.706	-9.363
700	10.439	48.667	43.611	3.539	28.667	25.186	-7.863
800	11.098	50.105	44.335	4.616	28.440	24.706	-6.749
900	11.648	51.445	45.051	5.755	28.251	24.254	-5.890
1000	12.102	52.696	45.753	6.943	28.083	23.817	-5.205
1100	12.477	53.868	46.439	8.172	27.924	23.396	-4.648
1200	12.788	54.967	47.104	9.436	27.769	22.988	-4.187
1300	13.047	56.002	47.750	10.728	27.609	22.601	-3.800
1400	13.264	56.977	48.374	12.044	27.441	22.223	-3.469
1500	13.447	57.898	48.978	13.380	27.261	21.848	-3.183
1527	13.489	58.138	49.138	13.744	27.210	21.756	-3.114
1527	13.489	58.138	49.138	13.744	26.599	21.756	-3.114
1560	13.541	58.427	49.331	14.190	26.535	21.644	-3.032
1560	13.541	58.427	49.331	14.190	23.616	21.644	-3.032
1600	13.603	58.771	49.563	14.733	23.565	21.595	-2.950
1700	13.735	59.600	50.129	16.100	23.441	21.466	-2.760
1800	13.849	60.388	50.677	17.479	23.319	21.348	-2.592
1900	13.948	61.140	51.209	18.869	23.199	21.259	-2.445
2000	14.034	61.858	51.724	20.268	23.079	21.157	-2.312

*Data estimated.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.442 + 3.348\times10^{-3}T - 1.939\times10^{5}T^{-2}$
$H°-H°_{298} = 8.442\times10^{-3}T + 1.674\times10^{-6}T^{2} + 1.939\times10^{2}T^{-1} - 3.316$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = 30.503 - 2.755\times10^{-3}T + 0.293\times10^{-6}T^{2} + 87.300T^{-1}$
$\Delta Gf° = 30.503 + 2.755\times10^{-3}T\ln T - 0.293\times10^{-6}T^{2} + 43.650T^{-1} - 25.659\times10^{-3}T$
1527-1560 K: $\Delta Hf° = 32.086 - 5.714\times10^{-3}T + 1.255\times10^{-6}T^{2} + 210.400T^{-1}$
$\Delta Gf° = 32.086 + 5.714\times10^{-3}T\ln T - 1.255\times10^{-6}T^{2} + 105.200T^{-1} - 46.946\times10^{-3}T$
1560-2000 K: $\Delta Hf° = 28.138 - 5.054\times10^{-3}T + 1.255\times10^{-6}T^{2} + 210.400T^{-1}$
$\Delta Gf° = 28.138 + 5.054\times10^{-3}T\ln T - 1.255\times10^{-6}T^{2} + 105.200T^{-1} - 39.562\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$BeN(g)$
Beryllium Nitride (ideal gas)
[Formation: $Be(c,l) + 0.5N_2(g) = BeN(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.192	49.872	49.872	0	102.000	94.631	-69.365
300	7.197	49.916	49.873	.013	102.000	94.584	-68.903
400	7.514	52.029	50.156	.749	101.951	92.119	-50.331
500	7.820	53.740	50.708	1.516	101.866	89.667	-39.193
600	8.069	55.188	51.336	2.311	101.759	87.242	-31.777
700	8.264	56.447	51.978	3.128	101.637	84.828	-26.484
800	8.414	57.561	52.609	3.962	101.502	82.436	-22.520
900	8.531	58.559	53.216	4.809	101.353	80.065	-19.442
1000	8.624	59.463	53.796	5.667	101.185	77.706	-16.982
1100	8.699	60.289	54.349	6.534	100.996	75.367	-14.974
1200	8.760	61.048	54.875	7.407	100.786	73.041	-13.302
1300	8.812	61.752	55.379	8.285	100.553	70.744	-11.893
1400	8.856	62.406	55.857	9.169	100.298	68.463	-10.687
1500	8.894	63.019	56.315	10.056	100.021	66.187	-9.643
1527	8.903	63.178	56.435	10.296	99.943	65.584	-9.387
1527	8.903	63.178	56.435	10.296	99.332	65.584	-9.387
1560	8.914	63.368	56.580	10.590	99.234	64.848	-9.085
1560	8.914	63.368	56.580	10.590	96.315	64.848	-9.085
1600	8.927	63.594	56.752	10.947	96.222	64.043	-8.748
1700	8.957	64.136	57.170	11.842	95.992	62.029	-7.974
1800	8.984	64.649	57.572	12.739	95.761	60.033	-7.289
1900	9.008	65.135	57.957	13.638	95.530	58.072	-6.680
2000	9.031	65.598	58.328	14.540	95.299	56.104	-6.131
2100	9.051	66.039	58.685	15.444	95.067	54.142	-5.635
2200	9.071	66.460	59.028	16.351	94.838	52.206	-5.186
2300	9.089	66.864	59.360	17.259	94.608	50.266	-4.776
2400	9.106	67.251	59.681	18.168	94.378	48.344	-4.402
2500	9.123	67.623	59.991	19.080	94.149	46.437	-4.059

*Data estimated.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 8.087 + 0.516\times10^{-3}T - 0.933\times10^{5}T^{-2}$
$H°-H°_{298} = 8.087\times10^{-3}T + 0.258\times10^{-6}T^{2} + 0.933\times10^{2}T^{-1} - 2.747$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = 102.149 + 0.087\times10^{-3}T - 0.998\times10^{-6}T^{2} - 25.850T^{-1}$
$\Delta Gf° = 102.149 - 0.087\times10^{-3}T\ln T + 0.998\times10^{-6}T^{2} - 12.925T^{-1} - 24.872\times10^{-3}T$
1527-1560 K: $\Delta Hf° = 103.733 - 2.872\times10^{-3}T - 0.037\times10^{-6}T^{2} + 97.250T^{-1}$
$\Delta Gf° = 103.733 + 2.872\times10^{-3}T\ln T + 0.037\times10^{-6}T^{2} + 48.625T^{-1} - 46.159\times10^{-3}T$
1560-2000 K: $\Delta Hf° = 99.784 - 2.211\times10^{-3}T - 0.037\times10^{-6}T^{2} + 97.250T^{-1}$
$\Delta Gf° = 99.784 + 2.211\times10^{-3}T\ln T + 0.037\times10^{-6}T^{2} + 48.625T^{-1} - 38.775\times10^{-3}T$
2000-2500 K: $\Delta Hf° = 101.121 - 3.276\times10^{-3}T + 0.230\times10^{-6}T^{2} - 452.700T^{-1}$
$\Delta Gf° = 101.121 + 3.276\times10^{-3}T\ln T - 0.230\times10^{-6}T^{2} - 226.350T^{-1} - 46.929\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$Be_3N_2(\alpha)$
α-Triberyllium Dinitride
[Formation: $3Be(c,l) + N_2(g) = Be_3N_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	15.490	8.226	8.226	0	-140.600	-127.376	93.368
300	15.601	8.322	8.226	.029	-140.605	-127.297	92.734
400	20.139	13.478	8.898	1.832	-140.807	-122.823	67.107
500	23.440	18.353	10.307	4.023	-140.822	-118.331	51.722
600	25.569	22.829	12.027	6.481	-140.712	-113.828	41.461
700	27.002	26.885	13.866	9.113	-140.532	-109.374	34.148
800	28.041	30.561	15.726	11.868	-140.314	-104.932	28.666
900	28.854	33.913	17.564	14.714	-140.078	-100.515	24.408
1000	29.536	36.989	19.354	17.635	-139.846	-96.137	21.010
1100	30.143	39.833	21.088	20.620	-139.635	-91.778	18.234
1200	30.707	42.480	22.762	23.662	-139.442	-87.452	15.927
1300*	31.152	44.955	24.374	26.755	-139.278	-83.105	13.971
1400	31.552	47.279	25.928	29.891	-139.147	-78.787	12.299
1500	31.894	49.468	27.426	33.063	-139.051	-74.511	10.856
1527	31.971	50.038	27.821	33.925	-139.032	-73.331	10.495
1527	31.971	50.038	27.821	33.925	-140.865	-73.331	10.495
1560	32.065	50.722	28.297	34.982	-140.846	-71.897	10.072
1560	32.065	50.722	28.297	34.982	-149.603	-71.897	10.072
1600	32.179	51.535	28.868	36.267	-149.499	-69.901	9.548

*Data extrapolated above 1200 K.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 24.513 + 5.704x10^{-3}T - 9.533x10^{5}T^{-2}$
$H°-H°_{298} = 24.513x10^{-3}T + 2.852x10^{-6}T^{2} + 9.533x10^{2}T^{-1} - 10.759$

Formation equations (kcal/mol):

298.15-1527 K: $ΔHf° = -143.655 + 3.773x10^{-3}T - 0.623x10^{-6}T^{2} + 591.900T^{-1}$
$ΔGf° = -143.655 - 3.773x10^{-3}TlnT + 0.623x10^{-6}T^{2} + 295.950T^{-1} + 72.582x10^{-3}T$
1527-1560 K: $ΔHf° = -138.904 - 5.104x10^{-3}T + 2.263x10^{-6}T^{2} + 961.200T^{-1}$
$ΔGf° = -138.904 + 5.104x10^{-3}TlnT - 2.263x10^{-6}T^{2} + 480.600T^{-1} + 8.720x10^{-3}T$
1560-1600 K: $ΔHf° = -150.750 - 3.124x10^{-3}T + 2.263x10^{-6}T^{2} + 961.200T^{-1}$
$ΔGf° = -150.750 + 3.124x10^{-3}TlnT - 2.263x10^{-6}T^{2} + 480.600T^{-1} + 30.872x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Furukawa (165). High-temperature data based on Douglas (125). Data extrapolated above 1200 K.

BeOH(g)
Beryllium Monohydroxide (ideal gas)
[Formation: $Be(c,l) + 0.5O_2(g) + 0.5H_2(g) = BeOH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	9.159	50.067	50.067	0	-27.400	-29.693	21.765
300	9.179	50.124	50.067	.017	-27.403	-29.708	21.642
400	10.113	52.899	50.439	.984	-27.574	-30.450	16.637
500	10.793	55.233	51.171	2.031	-27.743	-31.153	13.617
600	11.293	57.247	52.019	3.137	-27.910	-31.814	11.588
700	11.678	59.018	52.895	4.286	-28.076	-32.456	10.133
800	11.992	60.599	53.761	5.470	-28.242	-33.070	9.034
900	12.260	62.027	54.601	6.683	-28.408	-33.660	8.174
1000	12.495	63.331	55.410	7.921	-28.581	-34.236	7.482
1100	12.706	64.532	56.186	9.181	-28.765	-34.794	6.913
1200	12.896	65.646	56.929	10.461	-28.960	-35.339	6.436
1300	13.067	66.685	57.640	11.759	-29.169	-35.856	6.028
1400	13.221	67.659	58.320	13.074	-29.392	-36.360	5.676
1500	13.361	68.576	58.974	14.403	-29.631	-36.860	5.371
1527	13.395	68.815	59.146	14.764	-29.698	-36.984	5.293
1527	13.395	68.815	59.146	14.764	-30.309	-36.984	5.293
1560	13.436	69.101	59.353	15.208	-30.392	-37.135	5.202
1560	13.436	69.101	59.353	15.208	-33.311	-37.135	5.202
1600	13.486	69.442	59.601	15.746	-33.387	-37.230	5.085
1700	13.599	70.263	60.204	17.100	-33.571	-37.476	4.818
1800	13.701	71.044	60.786	18.465	-33.753	-37.706	4.578
1900	13.792	71.787	61.345	19.840	-33.931	-37.903	4.360
2000	13.875	72.496	61.885	21.223	-34.110	-38.109	4.164

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 10.737 + 1.820\times10^{-3}T - 1.885\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.737\times10^{-3}T + 0.910\times10^{-6}T^2 + 1.885\times10^{2}T^{-1} - 3.914$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf^\circ = -27.273 - 0.847\times10^{-3}T - 0.513\times10^{-6}T^2 + 51.050T^{-1}$
$\Delta Gf^\circ = -27.273 + 0.847\times10^{-3}T\ln T + 0.513\times10^{-6}T^2 + 25.525T^{-1} - 13.383\times10^{-3}T$
1527-1560 K: $\Delta Hf^\circ = -25.689 - 3.806\times10^{-3}T + 0.449\times10^{-6}T^2 + 174.150T^{-1}$
$\Delta Gf^\circ = -25.689 + 3.806\times10^{-3}T\ln T - 0.449\times10^{-6}T^2 + 87.075T^{-1} - 34.670\times10^{-3}T$
1560-2000 K: $\Delta Hf^\circ = -29.638 - 3.146\times10^{-3}T + 0.449\times10^{-6}T^2 + 174.150T^{-1}$
$\Delta Gf^\circ = -29.638 + 3.146\times10^{-3}T\ln T - 0.449\times10^{-6}T^2 + 87.075T^{-1} - 27.286\times10^{-3}T$

Source: Data from Chase (82) who estimated all except enthalpy of formation at 298 K.

$Be(OH)_2(g)$
Beryllium Dihydroxide (ideal gas)
[Formation: $Be(c,l) + O_2(g) + H_2(g) = Be(OH)_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.157	55.893	55.893	0	-161.700	-153.772	112.717
300	15.208	55.987	55.894	.028	-161.705	-153.724	111.987
400	17.385	60.684	56.519	1.666	-161.907	-151.030	82.518
500	18.792	64.725	57.765	3.480	-162.024	-148.298	64.820
600	19.773	68.243	59.225	5.411	-162.093	-145.541	53.013
700	20.512	71.348	60.739	7.426	-162.133	-142.784	44.578
800	21.112	74.128	62.243	9.508	-162.153	-140.018	38.251
900	21.626	76.645	63.705	11.646	-162.157	-137.247	33.328
1000	22.080	78.947	65.116	13.831	-162.155	-134.482	29.391
1100	22.489	81.071	66.471	16.060	-162.153	-131.715	26.169
1200	22.859	83.044	67.771	18.328	-162.152	-128.952	23.485
1300	23.194	84.887	69.017	20.631	-162.157	-126.178	21.212
1400	23.497	86.617	70.213	22.966	-162.170	-123.410	19.265
1500	23.770	88.248	71.362	25.329	-162.193	-120.652	17.579
1527	23.837	88.673	71.664	25.972	-162.201	-119.898	17.160
1527	23.837	88.673	71.664	25.972	-162.812	-119.898	17.160
1560	23.918	89.183	72.029	26.760	-162.823	-118.979	16.668
1560	23.918	89.183	72.029	26.760	-165.742	-118.979	16.668
1600	24.017	89.790	72.466	27.719	-165.729	-117.779	16.088
1700	24.240	91.253	73.528	30.132	-165.689	-114.793	14.757
1800	24.441	92.644	74.552	32.566	-165.644	-111.804	13.575
1900	24.622	93.971	75.540	35.019	-165.595	-108.798	12.514
2000	24.785	95.238	76.493	37.490	-165.542	-105.812	11.562

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.964 + 3.352x10^{-3}T - 4.273x10^{5}T^{-2}$
$H° - H°_{298} = 18.964x10^{-3}T + 1.676x10^{-6}T^{2} + 4.273x10^{2}T^{-1} - 7.236$

Formation equations (kcal/mol):

298.15-1527 K: $ΔHf° = -162.766 + 0.537x10^{-3}T - 0.208x10^{-6}T^{2} + 275.500T^{-1}$
$ΔGf° = -162.766 - 0.537x10^{-3}TlnT + 0.208x10^{-6}T^{2} + 137.750T^{-1} + 31.611x10^{-3}T$
1527-1560 K: $ΔHf° = -161.182 - 2.422x10^{-3}T + 0.754x10^{-6}T^{2} + 398.600T^{-1}$
$ΔGf° = -161.182 + 2.422x10^{-3}TlnT - 0.754x10^{-6}T^{2} + 199.300T^{-1} + 10.324x10^{-3}T$
1560-2000 K: $ΔHf° = -165.131 - 1.762x10^{-3}T + 0.754x10^{-6}T^{2} + 398.600T^{-1}$
$ΔGf° = -165.131 + 1.762x10^{-3}TlnT - 0.754x10^{-6}T^{2} + 199.300T^{-1} + 17.708x10^{-3}T$

Source: Data from Chase (82) who estimated all except enthalpy of formation at 298 K.

$BeSO_4(c)$
Beryllium Sulfate
[Reaction: $Be(c,l) + 0.5S_2(g) + 2O_2(g) = BeSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	20.482	18.635	18.635	0	-302.435	-269.967	197.889
300	20.581	18.762	18.635	.038	-302.437	-269.766	196.522
400	24.828	25.303	19.498	2.322	-302.408	-258.872	141.439
500	27.810	31.180	21.258	4.961	-302.145	-248.017	108.407
600	30.310	36.470	23.360	7.866	-301.719	-237.224	86.408
700	32.980	41.340	25.584	11.029	-301.118	-226.524	70.723
800	35.800	45.927	27.843	14.467	-300.309	-215.920	58.986
863	37.650	48.709	29.265	16.780	-299.682	-209.295	53.002
863*	37.650	49.017	29.265	17.046	-299.416	-209.295	53.002
900	38.730	50.620	30.110	18.459	-299.003	-205.439	49.887
908	38.970	50.964	30.292	18.770	-298.909	-204.608	49.247
908	38.970	56.110	30.292	23.443	-294.236	-204.608	49.247
1000	41.690	60.004	32.844	27.160	-293.037	-195.582	42.744
1100	43.759	64.080	35.501	31.437	-291.547	-185.909	36.936
1200	45.222	67.953	38.045	35.890	-289.924	-176.380	32.123
1300	46.258	71.616	40.488	40.466	-288.221	-166.982	28.072
1400	46.984	75.072	42.836	45.130	-286.471	-157.720	24.621
1500	47.480	78.331	45.094	49.855	-284.697	-148.596	21.650
1527	47.567	79.179	45.690	51.138	-284.218	-146.144	20.916
1527	47.567	79.179	45.690	51.138	-284.829	-146.144	20.916
1560	47.673	80.198	46.410	52.710	-284.243	-143.163	20.056
1560	47.673	80.198	46.410	52.710	-287.162	-143.163	20.056
1600	47.802	81.407	47.269	54.620	-286.424	-139.478	19.052
1700	47.970	84.310	49.363	59.410	-284.571	-130.360	16.759
1800	48.000	87.053	51.381	64.209	-282.724	-121.345	14.733
1900	48.000	89.649	53.328	69.009	-280.892	-112.414	12.930
2000	48.000	92.111	55.207	73.809	-279.073	-103.597	11.320

*Data above 863 K estimated except temperatures and enthalpies of transformation.

Phase changes:
863 K, α - β transition point of $BeSO_4$; ΔH° = 0.266 kcal/mol.
908 K, β - γ transition point of $BeSO_4$; ΔH° = 4.673 kcal/mol.
1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-863 K: $Cp^\circ = 17.885 + 22.876\times10^{-3}T - 3.757\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.885\times10^{-3}T + 11.438\times10^{-6}T^{2} + 3.757\times10^{2}T^{-1} - 7.609$
863-908 K: $Cp^\circ = 12.296 + 29.382\times10^{-3}T$
$H^\circ - H^\circ_{298} = 12.296\times10^{-3}T + 14.691\times10^{-6}T^{2} - 4.507$
908-2000 K: $Cp^\circ = 61.278 - 4.828\times10^{-3}T - 147.775\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 61.278\times10^{-3}T - 2.414\times10^{-6}T^{2} + 147.775\times10^{2}T^{-1} - 46.482$

Reaction equations (kcal/mol):

298.15-863 K: $\Delta Hr^\circ = -302.056 - 5.488\times10^{-3}T + 9.310\times10^{-6}T^{2} + 128.050T^{-1}$
$\Delta Gr^\circ = -302.056 + 5.488\times10^{-3}T\ln T - 9.310\times10^{-6}T^{2} + 64.025T^{-1} + 78.417\times10^{-3}T$
863-908 K: $\Delta Hr^\circ = -298.954 - 11.077\times10^{-3}T + 12.563\times10^{-6}T^{2} - 247.650T^{-1}$
$\Delta Gr^\circ = -298.954 + 11.077\times10^{-3}T\ln T - 12.563\times10^{-6}T^{2} - 123.825T^{-1} + 40.098\times10^{-3}T$
908-1527 K: $\Delta Hr^\circ = -340.929 + 37.905\times10^{-3}T - 4.542\times10^{-6}T^{2} + 14529.850T^{-1}$
$\Delta Gr^\circ = -340.929 - 37.905\times10^{-3}T\ln T + 4.542\times10^{-6}T^{2} + 7264.925T^{-1} + 395.461\times10^{-3}T$
1527-1560 K: $\Delta Hr^\circ = -339.345 + 34.947\times10^{-3}T - 3.580\times10^{-6}T^{2} + 14652.950T^{-1}$
$\Delta Gr^\circ = -339.345 - 34.947\times10^{-3}T\ln T + 3.580\times10^{-6}T^{2} + 7326.475T^{-1} + 374.174\times10^{-3}T$
1560-2000 K: $\Delta Hr^\circ = -343.294 + 35.606\times10^{-3}T - 3.580\times10^{-6}T^{2} + 14652.950T^{-1}$
$\Delta Gr^\circ = -343.294 - 35.606\times10^{-3}T\ln T + 3.580\times10^{-6}T^{2} + 7326.475T^{-1} + 381.558\times10^{-3}T$

Source: Data from DeKock (113) who estimated all above 863 K except temperatures and enthalpies of transformations.

$BeSO_4 \cdot H_2O(c)$
Beryllium Sulfate Monohydrate
[Reaction: $Be(c) + 0.5S_2(g) + 2.5O_2(g) + H_2(g) = BeSO_4 \cdot H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	28.560	28.910	28.910	0	-376.505	-330.491	242.253
300	28.726	29.087	28.910	.053	-376.511	-330.206	240.552
350	33.227	33.853	29.276	1.602	-376.597	-322.479	201.362
400	37.727	38.584	30.144	3.376	-376.492	-314.752	171.970
450	42.227	43.287	31.345	5.374	-376.200	-307.053	149.123
500	46.727	47.969	32.773	7.598	-375.712	-299.394	130.863
550	51.227	52.634	34.367	10.047	-375.029	-291.790	115.945

*Heat capacity at 298 K and all data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 1.914 + 89.652\times10^{-3}T - 0.074\times10^{5}T^{-2}$
$H° - H°_{298} = 1.914\times10^{-3}T + 44.826\times10^{-6}T^{2} + 0.074\times10^{2}T^{-1} - 4.580$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -370.014 - 31.530\times10^{-3}T + 42.028\times10^{-6}T^{2} - 246.350T^{-1}$
$\Delta Gr° = -370.014 + 31.530\times10^{-3}T\ln T - 42.028\times10^{-6}T^{2} - 123.175T^{-1} - 33.164\times10^{-3}T$

Source: Data from DeKock (113) who estimated heat capacity at 298 K and all data above 298 K.

$BeSO_4 \cdot 2H_2O(c)$
Beryllium Sulfate Dihydrate
[Reaction: $Be(c) + 0.5S_2(g) + 3O_2(g) + 2H_2(g) = BeSO_4 \cdot 2H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	36.630	39.010	39.010	0	-450.135	-390.522	286.257
300*	36.808	39.237	39.010	.068	-450.146	-390.153	284.222
350	41.383	45.261	39.475	2.025	-450.346	-380.136	237.364
400	45.506	51.061	40.563	4.199	-450.368	-370.102	202.212
450	49.175	56.637	42.041	6.568	-450.235	-360.077	174.875
500	52.392	61.988	43.770	9.109	-449.964	-350.072	153.014
550	55.155	67.115	45.662	11.799	-449.577	-340.098	135.141

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 28.114 + 53.796x10^{-3}T - 6.688x10^{5}T^{-2}$
$H°-H°_{298} = 28.114x10^{-3}T + 26.898x10^{-6}T^{2} + 6.688x10^{2}T^{-1} - 13.016$

Reaction equations (kcal/mol):

298.15-550 K: $ΔHr° = -448.998 - 15.401x10^{-3}T + 23.429x10^{-6}T^{2} + 408.950T^{-1}$
$ΔGr° = -448.998 + 15.401x10^{-3}T\ln T - 23.429x10^{-6}T^{2} + 204.475T^{-1} + 113.067x10^{-3}T$

Source: Data from DeKock (113) who estimated all above 298 K.

$BeSO_4 \cdot 4H_2O(c)$
Beryllium Sulfate Tetrahydrate
[Reaction: $Be(c) + 0.5S_2(g) + 4O_2(g) + 4H_2(g) = BeSO_4 \cdot 4H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	51.770	55.680	55.680	0	-593.735	-505.873	370.810
300	52.049	56.001	55.681	.096	-593.757	-505.328	368.127
350	59.503	64.586	56.343	2.885	-594.170	-490.553	306.311
400	66.829	73.011	57.901	6.044	-594.260	-475.740	259.929
450	74.025	81.299	60.041	9.566	-594.036	-460.938	223.859
500	81.091	89.465	62.575	13.445	-593.493	-446.174	195.020
550	88.028	97.520	65.387	17.673	-592.643	-431.478	171.451

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 12.637 + 138.396\times10^{-3}T - 1.893\times10^{5}T^{-2}$

$H°-H°_{298} = 12.637\times10^{-3}T + 69.198\times10^{-6}T^{2} + 1.893\times10^{2}T^{-1} - 10.554$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -583.970 - 51.020\times10^{-3}T + 64.388\times10^{-6}T^{2} - 82.750T^{-1}$

$\Delta Gr° = -583.970 + 51.020\times10^{-3}T\ln T - 64.388\times10^{-6}T^{2} - 41.375T^{-1} - 9.088\times10^{-3}T$

Source: Data from DeKock (113).

$Be_2SiO_4(c)$
Beryllium Orthosilicate, Phenacite
[Formation: $2Be(c,l) + Si(c,l) + 2O_2(g) = Be_2SiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	22.840	15.342	15.342	0	-485.800	-458.457	336.054
300*	22.968	15.483	15.343	.042	-485.807	-458.290	333.859
400	28.860	22.946	16.318	2.651	-485.997	-449.079	245.362
500	32.730	29.819	18.343	5.738	-485.920	-439.858	192.260
600	35.650	36.054	20.784	9.162	-485.668	-430.660	156.866
700	37.970	41.732	23.378	12.848	-485.279	-421.530	131.606
800	39.680	46.920	26.001	16.735	-484.789	-412.453	112.675
900	40.810	51.662	28.592	20.763	-484.243	-403.436	97.966
1000	41.600	56.005	31.120	24.885	-483.679	-394.484	86.213
1100	42.150	59.996	33.565	29.074	-483.129	-385.599	76.610
1200	42.590	63.683	35.923	33.312	-482.597	-376.765	68.617
1300	42.934	67.106	38.192	37.588	-482.095	-367.955	61.858
1400	43.240	70.300	40.374	41.897	-481.627	-359.189	56.071
1500	43.472	73.291	42.469	46.233	-481.192	-350.489	51.066
1527	43.534	74.067	43.021	47.408	-481.081	-348.126	49.824
1527	43.534	74.067	43.021	47.408	-482.303	-348.126	49.824
1560	43.610	74.999	43.687	48.846	-482.173	-345.246	48.367
1560	43.610	74.999	43.687	48.846	-488.011	-345.246	48.367
1600	43.702	76.104	44.484	50.592	-487.799	-341.585	46.658
1687	43.900	78.423	46.175	54.402	-487.334	-333.648	43.223
1687	43.900	78.423	46.175	54.402	-499.416	-333.648	43.223
1700	43.930	78.760	46.423	54.973	-499.337	-332.366	42.728
1800	44.156	81.277	48.289	59.378	-498.726	-322.565	39.164
1833	44.230	82.080	48.891	60.836	-498.523	-319.338	38.074

*Data above 298 K estimated.

Phase changes:
1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.
1833 K, incongruent melting point of Be_2SiO_4.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1833 K: $Cp° = 35.742 + 6.058 \times 10^{-3}T - 13.075 \times 10^{5}T^{-2}$
$H° - H°_{298} = 35.742 \times 10^{-3}T + 3.029 \times 10^{-6}T^{2} + 13.075 \times 10^{2}T^{-1} - 15.311$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = -490.529 + 6.121 \times 10^{-3}T - 0.252 \times 10^{-6}T^{2} + 872.400T^{-1}$
$\Delta Gf° = -490.529 - 6.121 \times 10^{-3}T\ln T + 0.252 \times 10^{-6}T^{2} + 436.200T^{-1} + 137.461 \times 10^{-3}T$
1527-1560 K: $\Delta Hf° = -487.361 + 0.203 \times 10^{-3}T + 1.672 \times 10^{-6}T^{2} + 1118.600T^{-1}$
$\Delta Gf° = -487.361 - 0.203 \times 10^{-3}T\ln T - 1.672 \times 10^{-6}T^{2} + 559.300T^{-1} + 94.886 \times 10^{-3}T$
1560-1687 K: $\Delta Hf° = -495.258 + 1.523 \times 10^{-3}T + 1.672 \times 10^{-6}T^{2} + 1118.600T^{-1}$
$\Delta Gf° = -495.258 - 1.523 \times 10^{-3}T\ln T - 1.672 \times 10^{-6}T^{2} + 559.300T^{-1} + 109.654 \times 10^{-3}T$
1687-1833 K: $\Delta Hf° = -507.688 + 1.102 \times 10^{-3}T + 2.023 \times 10^{-6}T^{2} + 1217.100T^{-1}$
$\Delta Gf° = -507.688 - 1.102 \times 10^{-3}T\ln T - 2.023 \times 10^{-6}T^{2} + 608.550T^{-1} + 114.468 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Other data from JANAF (127) who estimated all above 298 K.

BeWO$_4$(c)
Beryllium Tungstate
[Formation: Be(c,l) + W(c) + 2O$_2$(g) = BeWO$_4$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H$^\circ_{298}$)/T	H°- H$^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.250	21.120	21.120	0	-361.700	-335.773	246.125
300	23.350	21.264	21.121	.043	-361.701	-335.612	244.490
400	27.000	28.508	22.083	2.570	-361.621	-326.920	178.619
500	29.520	34.816	24.014	5.401	-361.359	-318.276	139.117
600	31.390	40.370	26.285	8.451	-360.982	-309.692	112.804
700	32.820	45.318	28.658	11.662	-360.528	-301.179	94.031
800	34.150	49.788	31.024	15.011	-360.005	-292.739	79.972
900	35.400	53.883	33.340	18.489	-359.413	-284.357	69.051
1000	36.570	57.674	35.586	22.088	-358.751	-276.055	60.331
1100	37.700	61.213	37.757	25.802	-358.030	-267.811	53.209
1200	38.780	64.539	39.851	29.626	-357.247	-259.655	47.289
1300	39.830	67.685	41.872	33.557	-356.403	-251.544	42.288
1400	40.900	70.676	43.824	37.593	-355.502	-243.502	38.012
1500	41.930	73.533	45.710	41.735	-354.535	-235.551	34.319
1527	42.219	74.284	46.208	42.871	-354.264	-233.405	33.405
1527	42.219	74.284	46.208	42.871	-354.875	-233.405	33.405
1560	42.572	75.190	46.812	44.270	-354.539	-230.790	32.332
1560	42.572	75.190	46.812	44.270	-357.458	-230.790	32.332
1600	43.000	76.273	47.535	45.981	-357.010	-227.546	31.081
1700	44.050	78.911	49.303	50.334	-355.827	-219.492	28.217
1800	45.100	81.459	51.020	54.791	-354.561	-211.524	25.682
1900	46.150	83.926	52.687	59.354	-353.208	-203.594	23.418
2000	47.200	86.319	54.308	64.021	-351.770	-195.764	21.392

*Data estimated.

Phase changes: 1527 K, α − β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 26.533 + 10.508\times10^{-3}T - 5.703\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 26.533\times10^{-3}T + 5.254\times10^{-6}T^{2} + 5.703\times10^{2}T^{-1} - 10.291$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf^\circ = -363.538 + 1.517\times10^{-3}T + 2.915\times10^{-6}T^{2} + 335.800T^{-1}$
$\Delta Gf^\circ = -363.538 - 1.517\times10^{-3}T\ln T - 2.915\times10^{-6}T^{2} + 167.900T^{-1} + 100.747\times10^{-3}T$
1527-1560 K: $\Delta Hf^\circ = -361.954 - 1.442\times10^{-3}T + 3.877\times10^{-6}T^{2} + 458.900T^{-1}$
$\Delta Gf^\circ = -361.954 + 1.442\times10^{-3}T\ln T - 3.877\times10^{-6}T^{2} + 229.450T^{-1} + 79.460\times10^{-3}T$
1560-2000 K: $\Delta Hf^\circ = -365.903 - 0.782\times10^{-3}T + 3.877\times10^{-6}T^{2} + 458.900T^{-1}$
$\Delta Gf^\circ = -365.903 + 0.782\times10^{-3}T\ln T - 3.877\times10^{-6}T^{2} + 229.450T^{-1} + 86.844\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

BiAs(g)
Bismuth Arsenide (ideal gas)
[Formation: $Bi(c,l) + As[\alpha, 1/4As_4(g)] = BiAs(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°$_{298}$)/T	H°- H°$_{298}$	ΔHf°	ΔGf°	
298.15*	8.620	62.270	62.270	0	49.800	37.822	-27.724
300	8.630	62.330	62.277	.016	49.794	37.746	-27.498
400	8.770	64.830	62.613	.887	49.444	33.782	-18.457
500	8.830	66.790	63.256	1.767	49.053	29.915	-13.076
544.59	8.848	67.545	63.577	2.161	48.858	28.215	-11.323
544.59	8.848	67.545	63.577	2.161	46.158	28.215	-11.323
600	8.870	68.410	63.990	2.652	45.903	26.395	-9.614
700	8.890	69.780	64.723	3.540	45.458	23.178	-7.237
800	8.910	70.970	65.433	4.430	45.017	20.028	-5.471
876	8.918	71.779	65.948	5.108	44.682	17.663	-4.407
876	8.918	71.779	65.948	5.108	36.373	17.663	-4.407
900	8.920	72.020	66.107	5.322	36.310	17.152	-4.165
1000	8.930	72.960	66.746	6.214	36.050	15.042	-3.287
1100	8.930	73.810	67.349	7.107	35.796	12.952	-2.573
1200	8.940	74.580	67.912	8.001	35.546	10.902	-1.985
1300	8.940	75.300	68.458	8.895	35.295	8.852	-1.488
1400	8.950	75.960	68.967	9.790	35.045	6.829	-1.066
1500	8.950	76.580	69.457	10.685	34.795	4.822	-.703

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 8.934 + 0.022 \times 10^{-3}T - 0.280 \times 10^{5}T^{-2}$
$H° - H°_{298} = 8.934 \times 10^{-3}T + 0.011 \times 10^{-6}T^{2} + 0.280 \times 10^{2}T^{-1} - 2.759$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = 49.847 - 0.080 \times 10^{-3}T - 3.762 \times 10^{-6}T^{2} + 92.700T^{-1}$
$\Delta Gf° = 49.847 + 0.080 \times 10^{-3}T\ln T + 3.762 \times 10^{-6}T^{2} + 46.350T^{-1} - 42.434 \times 10^{-3}T$
544.59-876 K: $\Delta Hf° = 47.071 - 2.610 \times 10^{-3}T - 0.719 \times 10^{-6}T^{2} + 393.300T^{-1}$
$\Delta Gf° = 47.071 + 2.610 \times 10^{-3}T\ln T + 0.719 \times 10^{-6}T^{2} + 196.650T^{-1} - 52.124 \times 10^{-3}T$
876-1500 K: $\Delta Hf° = 37.743 - 1.912 \times 10^{-3}T - 0.141 \times 10^{-6}T^{2} + 361.800T^{-1}$
$\Delta Gf° = 37.743 + 1.912 \times 10^{-3}T\ln T + 0.141 \times 10^{-6}T^{2} + 180.900T^{-1} - 36.219 \times 10^{-3}T$

Source: Data from Prusaczyk (410) who estimated molecular constants.

$BiAs_3(g)$
Bismuth Triarsenide (ideal gas)
[Formation: $Bi(c,l) + 3As[\alpha,1/4As_4(g)] = BiAs_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.100	87.910	87.910	0	42.900	28.366	-20.792
300	19.110	88.020	87.910	.035	42.891	28.278	-20.600
400	19.440	93.570	88.655	1.966	42.401	23.479	-12.828
500	19.600	97.930	90.094	3.918	41.856	18.812	-8.223
544.59	19.636	99.606	90.805	4.793	41.586	16.766	-6.728
544.59	19.636	99.606	90.805	4.793	38.886	16.766	-6.728
600	19.680	101.510	91.707	5.882	38.531	14.530	-5.292
700	19.730	104.550	93.331	7.853	37.889	10.579	-3.303
800	19.760	107.190	94.905	9.828	37.227	6.725	-1.837
876	19.775	108.985	96.051	11.330	36.707	3.839	-.958
876	19.775	108.985	96.051	11.330	11.780	3.839	-.958
900	19.780	109.520	96.403	11.805	11.741	3.622	-.880
1000	19.800	111.600	97.816	13.784	11.582	2.738	-.598
1100	19.810	113.490	99.158	15.765	11.428	1.857	-.369
1200	19.820	115.210	100.421	17.747	11.278	1.005	-.183
1300	19.830	116.800	101.623	19.730	11.126	.150	-.025
1400	19.840	118.270	102.761	21.713	10.974	-.691	.108
1500	19.840	119.640	103.842	23.697	10.823	-1.516	.221

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 19.863 + 0.006\times10^{-3}T - 0.676\times10^{5}T^{-2}$
$H°- H°_{298} = 19.863\times10^{-3}T + 0.003\times10^{-6}T^{2} + 0.676\times10^{2}T^{-1} - 6.149$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = 43.135 - 0.533\times10^{-3}T - 4.912\times10^{-6}T^{2} + 107.500T^{-1}$
$\Delta Gf° = 43.135 + 0.533\times10^{-3}T\ln T + 4.912\times10^{-6}T^{2} + 53.750T^{-1} - 54.642\times10^{-3}T$
544.59-876 K: $\Delta Hf° = 40.358 - 3.063\times10^{-3}T - 1.869\times10^{-6}T^{2} + 408.100T^{-1}$
$\Delta Gf° = 40.358 + 3.063\times10^{-3}T\ln T + 1.869\times10^{-6}T^{2} + 204.050T^{-1} - 64.332\times10^{-3}T$
876-1500 K: $\Delta Hf° = 12.374 - 0.969\times10^{-3}T - 0.135\times10^{-6}T^{2} + 313.600T^{-1}$
$\Delta Gf° = 12.374 + 0.969\times10^{-3}T\ln T + 0.135\times10^{-6}T^{2} + 156.800T^{-1} - 16.619\times10^{-3}T$

Source: Data from Prusaczyk (410) who estimated molecular constants.

$Bi_2As_2(g)$
Dibismuth Diarsenide (ideal gas)
[Formation: $2Bi(c,l) + 2As[\alpha, 1/4As_4(g)] = Bi_2As_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	19.210	91.480	91.480	0	50.300	36.200	-26.535
300	19.220	91.600	91.480	.036	50.292	36.114	-26.309
400	19.500	97.170	92.237	1.973	49.787	31.459	-17.188
500	19.630	101.540	93.678	3.931	49.203	26.947	-11.778
544.59	19.661	103.218	94.391	4.807	48.901	24.970	-10.021
544.59	19.661	103.218	94.391	4.807	43.501	24.970	-10.021
600	19.700	105.120	95.290	5.898	43.100	23.103	-8.415
700	19.750	108.170	96.926	7.871	42.407	19.821	-6.188
800	19.780	110.810	98.500	9.848	41.722	16.648	-4.548
876	19.795	112.605	99.647	11.351	41.199	14.277	-3.562
876	19.795	112.605	99.647	11.351	24.581	14.277	-3.562
900	19.800	113.140	100	11.826	24.502	13.995	-3.399
1000	19.810	115.220	101.413	13.807	24.179	12.863	-2.811
1100	19.820	117.110	102.757	15.788	23.866	11.740	-2.332
1200	19.830	118.840	104.031	17.771	23.561	10.656	-1.941
1300	19.840	120.420	105.225	19.754	23.254	9.601	-1.614
1400	19.840	121.890	106.363	21.738	22.948	8.559	-1.336
1500	19.850	123.260	107.445	23.723	22.643	7.547	-1.100

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 19.865 + 0.004x10^{-3}T - 0.585x10^{5}T^{-2}$
$H°- H^\circ_{298} = 19.865x10^{-3}T + 0.002x10^{-6}T^2 + 0.585x10^{2}T^{-1} - 6.119$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = 49.793 + 1.837x10^{-3}T - 7.544x10^{-6}T^2 + 187.900T^{-1}$
$\Delta Gf° = 49.793 - 1.837x10^{-3}T\ln T + 7.544x10^{-6}T^2 + 93.950T^{-1} - 38.430x10^{-3}T$
544.59-876 K: $\Delta Hf° = 44.239 - 3.223x10^{-3}T - 1.458x10^{-6}T^2 + 789.100T^{-1}$
$\Delta Gf° = 44.239 + 3.223x10^{-3}T\ln T + 1.458x10^{-6}T^2 + 394.550T^{-1} - 57.810x10^{-3}T$
876-1500 K: $\Delta Hf° = 25.583 - 1.827x10^{-3}T - 0.302x10^{-6}T^2 + 726.100T^{-1}$
$\Delta Gf° = 25.583 + 1.827x10^{-3}T\ln T + 0.302x10^{-6}T^2 + 363.050T^{-1} - 26.001x10^{-3}T$

Source: Data from Prusaczyk (410) who estimated molecular constants.

$Bi_3As(g)$
Tribismuth Arsenide (ideal gas)
[Formation: $3Bi(c,l) + As[\alpha, 1/4As_4(g)] = Bi_3As(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.420	95.060	95.060	0	50.900	37.231	-27.291
300	19.420	95.180	95.060	.036	50.892	37.149	-27.063
400	19.620	100.800	95.828	1.989	50.382	32.636	-17.831
500	19.710	105.190	97.278	3.956	49.762	28.274	-12.358
544.59	19.732	106.875	97.996	4.835	49.431	26.365	-10.580
544.59	19.732	106.875	97.996	4.835	41.331	26.365	-10.580
600	19.760	108.790	98.907	5.930	40.885	24.857	-9.054
700	19.790	111.830	100.534	7.907	40.143	22.252	-6.947
800	19.810	114.480	102.121	9.887	39.436	19.751	-5.396
876	19.818	116.274	103.268	11.393	38.914	17.892	-4.464
876	19.818	116.274	103.268	11.393	30.605	17.892	-4.464
900	19.820	116.810	103.622	11.869	30.485	17.546	-4.261
1000	19.830	118.900	105.049	13.851	29.997	16.149	-3.529
1100	19.840	120.790	106.395	15.835	29.528	14.780	-2.937
1200	19.840	122.520	107.671	17.819	29.068	13.472	-2.453
1300	19.850	124.110	108.877	19.803	28.607	12.187	-2.049
1400	19.850	125.580	110.017	21.788	28.147	10.935	-1.707
1500	19.850	126.950	111.101	23.773	27.687	9.729	-1.417

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 19.869 + 0.002\times10^{-3}T - 0.401\times10^{5}T^{-2}$
$H°-H°_{298} = 19.869\times10^{-3}T + 0.001\times10^{-6}T^{2} + 0.401\times10^{2}T^{-1} - 6.059$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = 49.681 + 4.209\times10^{-3}T - 10.176\times10^{-6}T^{2} + 259.000T^{-1}$
$\Delta Gf° = 49.681 - 4.209\times10^{-3}T\ln T + 10.176\times10^{-6}T^{2} + 129.500T^{-1} - 22.267\times10^{-3}T$
544.59-876 K: $\Delta Hf° = 41.351 - 3.381\times10^{-3}T - 1.047\times10^{-6}T^{2} + 1160.800T^{-1}$
$\Delta Gf° = 41.351 + 3.381\times10^{-3}T\ln T + 1.047\times10^{-6}T^{2} + 580.400T^{-1} - 51.337\times10^{-3}T$
876-1500 K: $\Delta Hf° = 32.023 - 2.683\times10^{-3}T - 0.469\times10^{-6}T^{2} + 1129.300T^{-1}$
$\Delta Gf° = 32.023 + 2.683\times10^{-3}T\ln T + 0.469\times10^{-6}T^{2} + 564.650T^{-1} - 35.433\times10^{-3}T$

Source: Data from Prusaczyk (410) who estimated molecular constants.

BiO(g)
Bismuth Monoxide (ideal gas)
[Formation: $Bi(c,l) + 0.5O_2(g) = BiO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.800	58.910	58.910	0	29.200	22.984	-16.848
300	7.810	58.960	58.913	.014	29.197	22.946	-16.716
400	8.170	61.260	59.225	.814	29.021	20.887	-11.412
500	8.400	63.110	59.822	1.644	28.827	18.877	-8.251
544.59	8.462	63.830	60.121	2.020	28.725	17.991	-7.220
544.59	8.462	63.830	60.121	2.020	26.025	17.991	-7.220
600	8.540	64.650	60.498	2.491	25.889	17.182	-6.258
700	8.640	65.980	61.194	3.350	25.665	15.745	-4.916
800	8.700	67.140	61.868	4.218	25.456	14.344	-3.919
900	8.750	68.160	62.504	5.090	25.255	12.969	-3.149
1000	8.780	69.090	63.123	5.967	25.059	11.614	-2.538
1100	8.810	69.930	63.705	6.847	24.867	10.275	-2.041
1200	8.830	70.690	64.249	7.729	24.675	8.971	-1.634

Phase change: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 8.500 + 0.362\times10^{-3}T - 0.718\times10^{5}T^{-2}$

$H°-H°_{298} = 8.500\times10^{-3}T + 0.181\times10^{-6}T^{2} + 0.718\times10^{2}T^{-1} - 2.791$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = 28.602 + 1.562\times10^{-3}T - 3.273\times10^{-6}T^{2} + 126.300T^{-1}$

$\Delta Gf° = 28.602 - 1.562\times10^{-3}T\ln T + 3.273\times10^{-6}T^{2} + 63.150T^{-1} - 11.627\times10^{-3}T$

544.59-1200 K: $\Delta Hf° = 25.825 - 0.968\times10^{-3}T - 0.230\times10^{-6}T^{2} + 426.900T^{-1}$

$\Delta Gf° = 25.825 + 0.968\times10^{-3}T\ln T + 0.230\times10^{-6}T^{2} + 213.450T^{-1} - 21.317\times10^{-3}T$

Source: Data from Sidorov (459).

$(BiO)_2(g)$
Dimeric Bismuth Monoxide (ideal gas)
[Formation: $2Bi(c,l) + O_2(g) = (BiO)_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	18.080	83.000	83.000	0	-7.800	-9.850	7.220
300	18.100	83.110	83.000	.033	-7.802	-9.860	7.183
400	18.480	88.420	83.717	1.881	-7.906	-10.534	5.755
500	19.140	92.660	85.104	3.778	-8.056	-11.175	4.885
544.59	19.234	94.299	85.791	4.634	-8.156	-11.455	4.597
544.59	19.234	94.299	85.791	4.634	-13.556	-11.455	4.597
600	19.350	96.170	86.665	5.703	-13.702	-11.238	4.093
700	19.480	99.160	88.239	7.645	-13.924	-10.805	3.373
800	19.570	101.770	89.772	9.598	-14.125	-10.341	2.825
900	19.630	104.070	91.228	11.558	-14.313	-9.859	2.394
1000	19.680	106.150	92.627	13.523	-14.493	-9.353	2.044
1100	19.710	108.020	93.936	15.492	-14.669	-8.828	1.754
1200	19.730	109.740	95.186	17.465	-14.844	-8.282	1.508

*Data except enthalpy of formation at 298 K estimated.

Phase change: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 19.555 + 0.262\text{x}10^{-3}T - 1.381\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.555\text{x}10^{-3}T + 0.131\text{x}10^{-6}T^2 + 1.381\text{x}10^{2}T^{-1} - 6.305$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf^\circ = -9.720 + 5.679\text{x}10^{-3}T - 6.776\text{x}10^{-6}T^2 + 247.100T^{-1}$

$\Delta Gf^\circ = -9.720 - 5.679\text{x}10^{-3}T\ln T + 6.776\text{x}10^{-6}T^2 + 123.550T^{-1} + 28.510\text{x}10^{-3}T$

544.59-1200 K: $\Delta Hf^\circ = -15.273 + 0.619\text{x}10^{-3}T - 0.690\text{x}10^{-6}T^2 + 848.300T^{-1}$

$\Delta Gf^\circ = -15.273 - 0.619\text{x}10^{-3}T\ln T + 0.690\text{x}10^{-6}T^2 + 424.150T^{-1} + 9.130\text{x}10^{-3}T$

Source: Data from Sidorov (459) who estimated molecular constants.

Bi_2O(linear,g)
Dibismuth Oxide (ideal gas)
[Formation: $2Bi(c,l) + 0.5O_2(g) = Bi_2O(linear,g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	12.990	70.530	70.530	0	21.700	16.063	-11.774
300	13.010	70.610	70.537	.022	21.694	16.028	-11.676
400	13.680	74.450	71.045	1.362	21.437	14.179	-7.747
500	14.060	77.550	72.056	2.747	21.140	12.395	-5.418
544.59	14.163	78.755	72.556	3.376	20.980	11.617	-4.662
544.59	14.163	78.755	72.556	3.376	15.580	11.617	-4.662
600	14.290	80.140	73.193	4.168	15.368	11.221	-4.087
700	14.440	82.350	74.346	5.603	15.028	10.560	-3.297
800	14.550	84.290	75.473	7.054	14.724	9.948	-2.717
900	14.620	86.010	76.552	8.512	14.441	9.355	-2.272
1000	14.670	87.550	77.568	9.982	14.179	8.824	-1.928
1100	14.710	88.950	78.546	11.444	13.916	8.289	-1.647
1200	14.740	90.230	79.462	12.922	13.670	7.806	-1.422

*Data except enthalpy of formation at 298 K estimated. Linear refers to molecular configuration.

Phase change: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 14.405 + 0.408\times10^{-3}T - 1.366\times10^{5}T^{-2}$

$H°-H°_{298} = 14.405\times10^{-3}T + 0.204\times10^{-6}T^{2} + 1.366\times10^{2}T^{-1} - 4.771$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = 20.138 + 4.144\times10^{-3}T - 6.451\times10^{-6}T^{2} + 268.200T^{-1}$

$\Delta Gf° = 20.138 - 4.144\times10^{-3}T\ln T + 6.451\times10^{-6}T^{2} + 134.100T^{-1} + 6.509\times10^{-3}T$

544.59-1200 K: $\Delta Hf° = 14.585 - 0.916\times10^{-3}T - 0.366\times10^{-6}T^{2} + 869.400T^{-1}$

$\Delta Gf° = 14.585 + 0.916\times10^{-3}T\ln T + 0.366\times10^{-6}T^{2} + 434.700T^{-1} - 12.871\times10^{-3}T$

Source: Data from Sidorov (459) who estimated molecular constants.

Bi_2O(bent,g)
Dibismuth Oxide (ideal gas)
[Formation: $2Bi(c,l) + 0.5O_2(g) = Bi_2O(bent,g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	12.110	75.720	75.720	0	26.800	19.615	-14.378
300	12.130	75.790	75.720	.022	26.793	19.574	-14.259
400	12.750	79.380	76.207	1.269	26.444	17.214	-9.405
500	13.110	82.260	77.134	2.563	26.056	14.956	-6.537
544.59	13.208	83.384	77.600	3.150	25.854	13.970	-5.606
544.59	13.208	83.384	77.600	3.150	20.454	13.970	-5.606
600	13.330	84.670	78.193	3.886	20.185	13.321	-4.852
700	13.470	86.740	79.274	5.226	19.751	12.210	-3.812
800	13.570	88.540	80.318	6.578	19.347	11.171	-3.052
900	13.640	90.150	81.330	7.938	18.966	10.155	-2.466
1000	13.690	91.590	82.286	9.304	18.601	9.206	-2.012
1100	13.720	92.890	83.185	10.675	18.246	8.286	-1.646
1200	13.750	94.090	84.049	12.049	17.896	7.401	-1.348

*Data except enthalpy of formation at 298 K estimated. Bent refers to molecular configuration.

Phase change: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 13.397 + 0.420\times10^{-3}T - 1.255\times10^{5}T^{-2}$

$H°- H°_{298} = 13.397\times10^{-3}T + 0.210\times10^{-6}T^{2} + 1.255\times10^{2}T^{-1} - 4.434$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = 25.576 + 3.136\times10^{-3}T - 6.445\times10^{-6}T^{2} + 257.100T^{-1}$

$\Delta Gf° = 25.576 - 3.136\times10^{-3}T\ln T + 6.445\times10^{-6}T^{2} + 128.550T^{-1} - 5.491\times10^{-3}T$

544.59-1200 K: $\Delta Hf° = 20.022 - 1.924\times10^{-3}T - 0.360\times10^{-6}T^{2} + 858.300T^{-1}$

$\Delta Gf° = 20.022 + 1.924\times10^{-3}T\ln T + 0.360\times10^{-6}T^{2} + 429.150T^{-1} - 24.871\times10^{-3}T$

Source: Data from Sidorov (459) who estimated molecular constants.

$Bi_2O_3(g)$
Dibismuth Trioxide (ideal gas)
[Formation: $2Bi(c,l) + 1.5O_2(g) = Bi_2O_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	22.080	81.770	81.770	0	-54.900	-49.278	36.121
300	22.120	81.910	81.773	.041	-54.901	-49.241	35.872
400	23.530	88.490	82.662	2.331	-54.917	-47.355	25.874
500	24.290	93.830	84.378	4.726	-54.935	-45.459	19.870
544.59	24.486	95.913	85.238	5.813	-54.970	-44.618	17.905
544.59	24.486	95.913	85.238	5.813	-60.370	-44.618	17.905
600	24.730	98.300	86.337	7.178	-60.431	-43.016	15.668
700	25.010	102.130	88.321	9.666	-60.497	-40.103	12.520
800	25.190	105.490	90.269	12.177	-60.539	-37.186	10.159
900	25.320	108.460	92.123	14.703	-60.568	-34.271	8.322
1000	25.420	111.130	93.890	17.240	-60.589	-31.334	6.848
1100	25.490	113.560	95.573	19.786	-60.608	-28.416	5.646
1200	25.540	115.780	97.165	22.338	-60.628	-25.477	4.640

*Data except enthalpy of formation at 298 K estimated.

Phase change: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 25.155 + 0.560x10^{-3}T - 2.882x10^{5}T^{-2}$
$H°- H°_{298} = 25.155x10^{-3}T + 0.280x10^{-6}T^{2} + 2.882x10^{2}T^{-1} - 8.491$

Formation equations (kcal/mol):

298.15-544.59 K: $ΔHf° = -57.830 + 7.664x10^{-3}T - 6.879x10^{-6}T^{2} + 374.600T^{-1}$
$ΔGf° = -57.830 - 7.664x10^{-3}TlnT + 6.879x10^{-6}T^{2} + 187.300T^{-1} + 68.193x10^{-3}T$
544.59-1200 K: $ΔHf° = -63.383 + 2.604x10^{-3}T - 0.793x10^{-6}T^{2} + 975.800T^{-1}$
$ΔGf° = -63.383 - 2.604x10^{-3}TlnT + 0.793x10^{-6}T^{2} + 487.900T^{-1} + 48.813x10^{-3}T$

Source: Data from Sidorov (459) who estimated molecular constants.

$(Bi_2O_3)_2(g)$
Dimeric Dibismuth Trioxide (ideal gas)
[Formation: $4Bi(c,l) + 3O_2(g) = (Bi_2O_3)_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	48.210	121.780	121.780	0	-196.700	-173.005	126.814
300	48.290	122.080	121.783	.089	-196.694	-172.854	125.922
400	51.140	136.410	123.718	5.077	-196.320	-164.968	90.133
500	52.640	148.000	127.452	10.274	-195.948	-157.166	68.697
544.59	53.028	152.513	129.322	12.630	-195.837	-153.723	61.690
544.59	53.028	152.513	129.322	12.630	-206.637	-153.723	61.690
600	53.510	157.680	131.707	15.584	-206.535	-148.352	54.037
700	54.050	165.970	136.021	20.964	-206.261	-138.670	43.294
800	54.410	173.210	140.225	26.388	-205.943	-129.023	35.247
900	54.660	179.640	144.260	31.842	-205.599	-119.454	29.007
1000	54.840	185.400	148.082	37.318	-205.240	-109.870	24.012
1100	54.980	190.640	151.723	42.809	-204.878	-100.367	19.941
1200	55.080	195.430	155.168	48.314	-204.517	-90.860	16.548

*Data except enthalpy of formation at 298 K estimated.

Phase change: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 54.435 + 1.036\times10^{-3}T - 5.808\times10^{5}T^{-2}$

$H°-H°_{298} = 54.435\times10^{-3}T + 0.518\times10^{-6}T^{2} + 5.808\times10^{2}T^{-1} - 18.224$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = -203.801 + 19.453\times10^{-3}T - 13.799\times10^{-6}T^{2} + 753.600T^{-1}$

$\Delta Gf° = -203.801 - 19.453\times10^{-3}T\ln T + 13.799\times10^{-6}T^{2} + 376.800T^{-1} + 205.774\times10^{-3}T$

544.59-1200 K: $\Delta Hf° = -214.907 + 9.333\times10^{-3}T - 1.627\times10^{-6}T^{2} + 1956.000T^{-1}$

$\Delta Gf° = -214.907 - 9.333\times10^{-3}T\ln T + 1.627\times10^{-6}T^{2} + 978.000T^{-1} + 167.014\times10^{-3}T$

Source: Data from Sidorov (459) who estimated molecular constants.

$Bi_3O_4(g)$
Tribismuth Tetroxide (ideal gas)
[Formation: $3Bi(c,l) + 2O_2(g) = Bi_3O_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	32.500	103.270	103.270	0	-100.600	-90.040	66.000
300	32.750	103.470	103.270	.060	-100.599	-89.971	65.543
400	34.570	113.140	104.570	3.428	-100.514	-86.442	47.229
500	35.630	120.980	107.094	6.943	-100.435	-82.929	36.248
544.59	35.456	124.016	108.357	8.528	-100.451	-81.375	32.656
544.59	35.456	124.016	108.357	8.528	-108.551	-81.375	32.656
600	35.240	127.550	109.985	10.539	-108.573	-78.625	28.639
700	36.630	133.150	112.887	14.184	-108.563	-73.618	22.984
800	36.880	138.060	115.735	17.860	-108.517	-68.621	18.746
900	37.060	142.420	118.467	21.558	-108.448	-63.657	15.458
1000	37.190	146.330	121.060	25.270	-108.367	-58.667	12.821
1100	37.290	149.880	123.521	28.995	-108.279	-53.708	10.671
1200	37.360	153.130	125.858	32.727	-108.193	-48.738	8.876

*Data except enthalpy of formation at 298 K estimated.

Phase change: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 36.932 + 0.678\times10^{-3}T - 4.120\times10^{5}T^{-2}$
$H° - H°_{298} = 36.932\times10^{-3}T + 0.339\times10^{-6}T^{2} + 4.120\times10^{2}T^{-1} - 12.423$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = -105.269 + 12.503\times10^{-3}T - 10.273\times10^{-6}T^{2} + 552.900T^{-1}$
$\Delta Gf° = -105.269 - 12.503\times10^{-3}T\ln T + 10.273\times10^{-6}T^{2} + 276.450T^{-1} + 116.144\times10^{-3}T$
544.59-1200 K: $\Delta Hf° = -113.599 + 4.913\times10^{-3}T - 1.144\times10^{-6}T^{2} + 1454.700T^{-1}$
$\Delta Gf° = -113.599 - 4.913\times10^{-3}T\ln T + 1.144\times10^{-6}T^{2} + 727.350T^{-1} + 87.074\times10^{-3}T$

Source: Data from Sidorov (459) who estimated molecular constants.

$Bi_2Se_3(c,l)$
Dibismuth Triselenide
[Reaction: $2Bi(c,l) + 1.5Se_2(g) = Bi_2Se_3(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	29.700	57.300	57.300	0	-83.450	-66.420	48.686
300	29.710	57.480	57.313	.050	-83.449	-66.316	48.311
400	30.170	66.090	58.465	3.050	-83.184	-60.643	33.134
500	30.630	72.880	60.700	6.090	-82.972	-55.034	24.055
544.59	30.835	75.505	61.806	7.460	-82.899	-52.551	21.089
544.59	30.835	75.505	61.806	7.460	-88.299	-52.551	21.089
600	31.090	78.500	63.217	9.170	-88.224	-48.927	17.821
700	31.550	83.330	65.744	12.310	-87.985	-42.383	13.233
800	32.010	87.570	68.220	15.480	-87.683	-35.883	9.803
900	32.470	91.370	70.581	18.710	-87.293	-29.441	7.149
995	32.910	94.650	72.728	21.810	-86.869	-23.352	5.129
995*	45.000	115.450	72.728	42.510	-66.169	-23.352	5.129
1000	45.000	115.680	72.950	42.730	-66.090	-23.145	5.058
1100	45.000	119.970	77.034	47.230	-64.387	-18.934	3.762

*Heat capacity of liquid estimated.

Phase changes: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
995 K, melting point of Bi_2Se_3; ΔH° = 20.700 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-995 K: $Cp° = 28.444 + 4.446x10^{-3}T - 0.062x10^{5}T^{-2}$
$H°-H°_{298} = 28.444x10^{-3}T + 2.223x10^{-6}T^{2} + 0.062x10^{2}T^{-1} - 8.699$
995-1100 K: $Cp° = 45.000$
$H°-H°_{298} = 45.000x10^{-3}T - 2.265$

Reaction equations (kcal/mol):

298.15-544.59 K: $ΔHr° = -85.087 + 5.802x10^{-3}T - 3.702x10^{-6}T^{2} + 70.550T^{-1}$
$ΔGr° = -85.087 - 5.802x10^{-3}TlnT + 3.702x10^{-6}T^{2} + 35.275T^{-1} + 94.168x10^{-3}T$
544.59-995 K: $ΔHr° = -90.641 + 0.742x10^{-3}T + 2.384x10^{-6}T^{2} + 671.750T^{-1}$
$ΔGr° = -90.641 - 0.742x10^{-3}TlnT - 2.384x10^{-6}T^{2} + 335.875T^{-1} + 74.788x10^{-3}T$
995-1100 K: $ΔHr° = -84.207 + 17.298x10^{-3}T + 0.161x10^{-6}T^{2} + 665.550T^{-1}$
$ΔGr° = -84.207 - 17.298x10^{-3}TlnT - 0.161x10^{-6}T^{2} + 332.775T^{-1} + 180.395x10^{-3}T$

Source: Data from Mills (332) who estimated heat capacity of liquid.

$Bi_2Te_3(c,l)$
Dibismuth Tritelluride
[Reaction: $2Bi(c,l) + 1.5Te_2(g) = Bi_2Te_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	29.740	62.400	62.400	0	-76.295	-59.144	43.353
300	29.750	62.580	62.400	.055	-76.286	-59.036	43.007
400	31.090	71.340	63.585	3.102	-75.800	-53.362	29.155
500	32.410	78.420	65.866	6.277	-75.285	-47.807	20.896
544.59	32.999	81.214	67.010	7.735	-75.056	-45.372	18.208
544.59	32.999	81.214	67.010	7.735	-80.456	-45.372	18.208
600	33.730	84.450	68.477	9.584	-80.163	-41.817	15.232
700	35.050	89.750	71.146	13.023	-79.504	-35.477	11.076
800	36.370	94.510	73.768	16.594	-78.708	-29.232	7.986
850	37.030	96.740	75.059	18.429	-78.259	-26.169	6.728
850	40	130.340	75.059	46.989	-49.699	-26.169	6.728
900	40	132.630	78.198	48.989	-49.088	-24.806	6.024
1000	40	136.840	83.851	52.989	-47.873	-22.158	4.843

Phase changes: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
850 K, melting point of Bi_2Te_3; ΔH° = 28.560 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-850 K: $Cp° = 26.001 + 12.956\times10^{-3}T - 0.110\times10^{5}T^{-2}$
$H°- H°_{298} = 26.001\times10^{-3}T + 6.478\times10^{-6}T^{2} + 0.110\times10^{2}T^{-1} - 8.365$
850-1000 K: $Cp° = 40$
$H°- H°_{298} = 40 \quad \times10^{-3}T + 12.989$

Reaction equations (kcal/mol):

298.15-544.59 K: $ΔHr° = -78.580 + 6.456\times10^{-3}T - 0.815\times10^{-6}T^{2} + 128.900T^{-1}$
$ΔGr° = -78.580 - 6.456\times10^{-3}T\ln T + 0.815\times10^{-6}T^{2} + 64.450T^{-1} + 101.007\times10^{-3}T$
544.59-850 K: $ΔHr° = -84.133 + 1.396\times10^{-3}T + 5.271\times10^{-6}T^{2} + 730.100T^{-1}$
$ΔGr° = -84.133 - 1.396\times10^{-3}T\ln T - 5.271\times10^{-6}T^{2} + 365.050T^{-1} + 81.627\times10^{-3}T$
850-1000 K: $ΔHr° = -62.779 + 15.395\times10^{-3}T - 1.207\times10^{-6}T^{2} + 719.100T^{-1}$
$ΔGr° = -62.779 - 15.395\times10^{-3}T\ln T + 1.207\times10^{-6}T^{2} + 359.550T^{-1} + 145.432\times10^{-3}T$

Source: Data from Mills (332).

$CH(g)$
Carbon Monohydride (ideal gas)
[Formation: $C(c) + 0.5H_2(g) = CH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	6.972	43.721	43.721	0	142.000	134.026	-98.242
300	6.972	43.764	43.721	.013	142.003	133.976	-97.600
400	6.984	45.771	43.993	.711	142.109	131.284	-71.729
500	7.027	47.333	44.511	1.411	142.143	128.571	-56.198
600	7.112	48.621	45.093	2.117	142.122	125.858	-45.843
700	7.240	49.727	45.677	2.835	142.065	123.152	-38.449
800	7.401	50.704	46.246	3.566	141.984	120.455	-32.906
900	7.586	51.586	46.790	4.316	141.891	117.769	-28.598
1000	7.783	52.395	47.311	5.084	141.794	115.094	-25.153
1100	7.985	53.146	47.808	5.872	141.694	112.439	-22.339
1200	8.186	53.850	48.282	6.681	141.598	109.773	-19.992
1300	8.380	54.513	48.737	7.509	141.503	107.124	-18.009
1400	8.564	55.141	49.172	8.357	141.413	104.483	-16.310
1500	8.735	55.737	49.589	9.222	141.327	101.849	-14.839
1600	8.893	56.306	49.992	10.103	141.245	99.220	-13.553
1700	9.036	56.850	50.379	11.000	141.167	96.595	-12.418
1800	9.165	57.370	50.753	11.910	141.092	93.976	-11.410
1900	9.280	57.869	51.115	12.832	141.018	91.359	-10.509
2000	9.382	58.347	51.464	13.766	140.947	88.750	-9.698

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 5.952 + 1.798\times10^{-3}T + 0.431\times10^{5}T^{-2}$

$H°-H°_{298} = 5.952\times10^{-3}T + 0.899\times10^{-6}T^{2} - 0.431\times10^{2}T^{-1} - 1.710$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 142.938 - 0.794\times10^{-3}T - 0.077\times10^{-6}T^{2} - 207.150T^{-1}$

$\Delta Gf° = 142.938 + 0.794\times10^{-3}T\ln T + 0.077\times10^{-6}T^{2} - 103.575T^{-1} - 33.274\times10^{-3}T$

Source: Data from JANAF (127).

$CH_2(g)$
Carbon Dihydride (ideal gas)
[Formation: $C(c) + H_2(g) = CH_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.269	46.324	46.324	0	92.350	88.252	-64.690
300	8.276	46.375	46.325	.015	92.348	88.226	-64.272
400	8.638	48.805	46.653	.861	92.256	86.866	-47.461
500	9.002	50.772	47.286	1.743	92.122	85.533	-37.386
600	9.370	52.445	48.010	2.661	91.963	84.230	-30.680
700	9.753	53.918	48.751	3.617	91.793	82.953	-25.899
800	10.144	55.246	49.481	4.612	91.623	81.703	-22.320
900	10.528	56.463	50.190	5.646	91.459	80.472	-19.541
1000	10.892	57.592	50.875	6.717	91.305	79.258	-17.322
1100	11.228	58.646	51.534	7.823	91.161	78.071	-15.511
1200	11.531	59.636	52.168	8.962	91.026	76.878	-14.001
1300	11.802	60.570	52.778	10.129	90.897	75.704	-12.727
1400	12.042	61.453	53.367	11.321	90.774	74.540	-11.636
1500	12.252	62.291	53.934	12.536	90.654	73.385	-10.692
1600	12.438	63.088	54.481	13.771	90.538	72.237	-9.867
1700	12.601	63.847	55.010	15.023	90.421	71.097	-9.140
1800	12.745	64.572	55.522	16.290	90.304	69.962	-8.494
1900	12.873	65.264	56.016	17.571	90.187	68.837	-7.918
2000	12.987	65.928	56.496	18.864	90.067	67.715	-7.399
2100	13.088	66.564	56.960	20.168	89.946	66.600	-6.931
2200	13.179	67.175	57.410	21.482	89.822	65.490	-6.506
2300	13.261	67.762	57.847	22.804	89.695	64.390	-6.118
2400	13.336	68.328	58.272	24.134	89.564	63.294	-5.764
2500	13.403	68.874	58.686	25.471	89.431	62.201	-5.438

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 8.580 + 2.242\times10^{-3}T - 0.870\times10^{5}T^{-2}$

$H°-H°_{298} = 8.580\times10^{-3}T + 1.121\times10^{-6}T^{2} + 0.870\times10^{2}T^{-1} - 2.950$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 93.002 - 1.394\times10^{-3}T - 0.064\times10^{-6}T^{2} - 68.800T^{-1}$

$\Delta Gf° = 93.002 + 1.394\times10^{-3}T\ln T + 0.064\times10^{-6}T^{2} - 34.400T^{-1} - 23.507\times10^{-3}T$

2000-2500 K: $\Delta Hf° = 94.994 - 3.517\times10^{-3}T + 0.568\times10^{-6}T^{2} - 616.500T^{-1}$

$\Delta Gf° = 94.994 + 3.517\times10^{-3}T\ln T - 0.568\times10^{-6}T^{2} - 308.250T^{-1} - 39.307\times10^{-3}T$

Source: Data from Chase (83).

$CH_3(g)$
Carbon Trihydride (ideal gas)
[Formation: $C(c) + 1.5H_2(g) = CH_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	9.248	46.381	46.381	0	34.820	35.357	-25.917
300	9.262	46.438	46.381	.017	34.813	35.360	-25.759
400	10.048	49.210	46.752	.983	34.495	35.592	-19.446
500	10.815	51.536	47.484	2.026	34.172	35.902	-15.693
600	11.541	53.572	48.332	3.144	33.863	36.278	-13.214
700	12.231	55.404	49.214	4.333	33.575	36.703	-11.459
800	12.888	57.080	50.094	5.589	33.313	37.169	-10.154
900	13.510	58.634	50.956	6.910	33.081	37.664	-9.146
1000	14.090	60.088	51.798	8.290	32.877	38.184	-8.345
1100	14.624	61.456	52.614	9.726	32.700	38.734	-7.696
1200	15.109	62.750	53.406	11.213	32.545	39.280	-7.154
1300	15.547	63.977	54.172	12.746	32.409	39.846	-6.699
1400	15.939	65.144	54.915	14.321	32.291	40.422	-6.310
1500	16.289	66.256	55.634	15.933	32.184	41.006	-5.975
1600	16.602	67.317	56.331	17.578	32.090	41.598	-5.682
1700	16.880	68.332	57.007	19.252	32.001	42.196	-5.425
1800	17.129	69.304	57.663	20.953	31.919	42.798	-5.196
1900	17.350	70.236	58.301	22.677	31.843	43.405	-4.993
2000	17.548	71.131	58.920	24.422	31.767	44.016	-4.810
2100	17.726	71.992	59.522	26.186	31.694	44.629	-4.645
2200	17.885	72.820	60.108	27.966	31.620	45.244	-4.495
2300	18.028	73.618	60.678	29.762	31.548	45.868	-4.358
2400	18.157	74.389	61.234	31.571	31.473	46.491	-4.234
2500	18.274	75.132	61.775	33.393	31.399	47.120	-4.119

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp^\circ = 10.166 + 3.788\text{x}10^{-3}T - 1.819\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.166\text{x}10^{-3}T + 1.894\text{x}10^{-6}T^2 + 1.819\text{x}10^{2}T^{-1} - 3.809$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 35.566 - 3.036\text{x}10^{-3}T + 0.499\text{x}10^{-6}T^2 + 34.350T^{-1}$

$\Delta Gf^\circ = 35.566 + 3.036\text{x}10^{-3}T\ln T - 0.499\text{x}10^{-6}T^2 + 17.175T^{-1} - 18.041\text{x}10^{-3}T$

2000-2500 K: $\Delta Hf^\circ = 37.557 - 5.159\text{x}10^{-3}T + 1.132\text{x}10^{-6}T^2 - 513.350T^{-1}$

$\Delta Gf^\circ = 37.557 + 5.159\text{x}10^{-3}T\ln T - 1.132\text{x}10^{-6}T^2 - 256.675T^{-1} - 33.842\text{x}10^{-3}T$

Source: Data from JANAF (127).

$CH_4(g)$
Methane (ideal gas)
Formation: $C(c) + 2H_2(g) = CH_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.518	44.490	44.490	0	-17.880	-12.127	8.889
300	8.535	44.543	44.490	.016	-17.894	-12.091	8.808
400	9.680	47.144	44.837	.923	-18.619	-10.046	5.489
500	11.076	49.453	45.533	1.960	-19.297	-7.824	3.420
600	12.483	51.597	46.367	3.138	-19.896	-5.471	1.993
700	13.813	53.622	47.259	4.454	-20.408	-3.026	.945
800	15.041	55.548	48.177	5.897	-20.836	-.512	.140
900	16.157	57.385	49.098	7.458	-21.184	2.049	-.497
1000	17.160	59.141	50.016	9.125	-21.460	4.644	-1.015
1100	18.052	60.819	50.922	10.887	-21.674	7.277	-1.446
1200	18.842	62.424	51.814	12.732	-21.839	9.907	-1.804
1300	19.538	63.960	52.689	14.652	-21.961	12.558	-2.111
1400	20.150	65.431	53.547	16.637	-22.047	15.215	-2.375
1500	20.688	66.840	54.387	18.679	-22.107	17.879	-2.605
1600	21.161	68.191	55.209	20.772	-22.142	20.544	-2.806
1700	21.579	69.486	56.010	22.910	-22.160	23.216	-2.985
1800	21.947	70.730	56.793	25.086	-22.165	25.884	-3.143
1900	22.273	71.926	57.559	27.298	-22.157	28.554	-3.284
2000	22.562	73.076	58.306	29.540	-22.143	31.223	-3.412

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.631 + 8.928\times10^{-3}T - 1.578\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 7.631\times10^{-3}T + 4.464\times10^{-6}T^{2} + 1.578\times10^{2}T^{-1} - 3.201$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -15.573 - 8.799\times10^{-3}T + 2.860\times10^{-6}T^{2} + 18.500T^{-1}$
$\Delta Gf^\circ = -15.573 + 8.799\times10^{-3}T\ln T - 2.860\times10^{-6}T^{2} + 9.250T^{-1} - 37.827\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data from JANAF (127).

$C_2H_2(g)$
Acetylene (ideal gas)
[Formation: $2C(c) + H_2(g) = C_2H_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.539	48.004	48.004	0	54.190	50.000	-36.651
300	10.571	48.069	48.004	.020	54.189	49.974	-36.406
400	12.065	51.326	48.438	1.155	54.142	48.577	-26.541
500	13.114	54.139	49.303	2.418	54.072	47.192	-20.628
600	13.931	56.604	50.319	3.771	53.971	45.827	-16.692
700	14.615	58.805	51.378	5.199	53.849	44.477	-13.886
800	15.239	60.798	52.432	6.693	53.719	43.149	-11.787
900	15.801	62.625	53.464	8.245	53.586	41.833	-10.158
1000	16.318	64.317	54.465	9.852	53.461	40.534	-8.859
1100	16.789	65.895	55.434	11.507	53.342	39.268	-7.802
1200	17.221	67.375	56.368	13.208	53.231	37.972	-6.916
1300	17.613	68.769	57.269	14.950	53.127	36.704	-6.170
1400	17.968	70.087	58.138	16.729	53.032	35.444	-5.533
1500	18.291	71.338	58.976	18.543	52.943	34.192	-4.982
1600	18.582	72.528	59.786	20.387	52.862	32.945	-4.500
1700	18.845	73.663	60.570	22.258	52.782	31.700	-4.075
1800	19.085	74.747	61.328	24.155	52.708	30.464	-3.699
1900	19.302	75.785	62.062	26.074	52.637	29.229	-3.362
2000	19.504	76.780	62.772	28.015	52.567	28.001	-3.060

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.422 + 3.944\times10^{-3}T - 2.720\times10^{5}T^{-2}$

$H° - H°_{298} = 12.422\times10^{-3}T + 1.972\times10^{-6}T^{2} + 2.720\times10^{2}T^{-1} - 4.791$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 54.695 - 1.070\times10^{-3}T + 0.021\times10^{-6}T^{2} - 56.100T^{-1}$

$\Delta Gf° = 54.695 + 1.070\times10^{-3}T\ln T - 0.021\times10^{-6}T^{2} - 28.050T^{-1} - 21.522\times10^{-3}T$

Source: Data from JANAF (127).

$C_2H_4(g)$
Ethylene (ideal gas)
[Formation: $2C(c) + 2H_2(g) = C_2H_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.250	52.396	52.396	0	12.540	16.345	-11.981
300	10.292	52.459	52.396	.019	12.525	16.368	-11.924
400	12.679	55.745	52.827	1.167	11.797	17.763	-9.705
500	14.933	58.821	53.721	2.550	11.148	19.330	-8.449
600	16.889	61.721	54.816	4.143	10.587	21.022	-7.657
700	18.574	64.454	56.000	5.918	10.110	22.798	-7.118
800	20.039	67.033	57.219	7.851	9.713	24.640	-6.731
900	21.320	69.468	58.446	9.920	9.386	26.524	-6.441
1000	22.443	71.774	59.665	12.109	9.125	28.441	-6.216
1100	23.427	73.960	60.865	14.404	8.920	30.405	-6.041
1200	24.290	76.036	62.044	16.791	8.759	32.346	-5.891
1300	25.044	78.011	63.197	19.258	8.634	34.315	-5.769
1400	25.706	79.892	64.323	21.797	8.543	36.294	-5.666
1500	26.285	81.686	65.421	24.397	8.473	38.278	-5.577
1600	26.794	83.399	66.492	27.051	8.425	40.267	-5.500
1700	27.242	85.037	67.535	29.753	8.389	42.258	-5.433
1800	27.636	86.605	68.551	32.498	8.366	44.253	-5.373
1900	27.986	88.109	69.541	35.279	8.351	46.247	-5.319
2000	28.296	89.552	70.505	38.094	8.340	48.244	-5.272

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.657 + 8.460\times10^{-3}T - 5.270\times10^{5}T^{-2}$
$H° - H°_{298} = 13.657\times10^{-3}T + 4.230\times10^{-6}T^{2} + 5.270\times10^{2}T^{-1} - 6.215$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 13.528 - 6.291\times10^{-3}T + 1.860\times10^{-6}T^{2} + 215.400T^{-1}$
$\Delta Gf° = 13.528 + 6.291\times10^{-3}T\ln T - 1.860\times10^{-6}T^{2} + 107.700T^{-1} - 27.052\times10^{-3}T$

Source: Data from JANAF (127).

$C_2H_6(g)$
Ethane (ideal gas)
[Formation: $2C(c) + 3H_2(g) = C_2H_6(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.580	54.850	54.850	0	-20.240	-7.862	5.763
300	12.640	54.930	54.850	.030	-20.257	-7.780	5.668
400	15.680	58.990	55.390	1.440	-21.417	-3.450	1.885
500	18.660	62.810	56.490	3.160	-22.428	1.163	-.508
600	21.350	66.460	57.843	5.170	-23.272	5.968	-2.174
700	23.720	69.930	59.330	7.420	-23.976	10.894	-3.401
800	25.830	73.240	60.865	9.900	-24.532	15.915	-4.348
900	27.690	76.390	62.412	12.580	-24.959	20.999	-5.099
1000	29.330	79.390	63.960	15.430	-25.277	26.123	-5.709

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 9.223 + 20.996x10^{-3}T - 2.580x10^{5}T^{-2}$
$H°- H°_{298} = 9.223x10^{-3}T + 10.498x10^{-6}T^{2} + 2.580x10^{2}T^{-1} - 4.548$

Formation equations (kcal/mol):

298.15-1000 K: $ΔHf° = -15.678 - 17.181x10^{-3}T + 7.709x10^{-6}T^{2} - 37.100T^{-1}$
$ΔGf° = -15.678 + 17.181x10^{-3}T\ln T - 7.709x10^{-6}T^{2} - 18.550T^{-1} - 69.168x10^{-3}T$

Source: Data from Stull (479).

$C_6H_6(g)$
Benzene (ideal gas)
[Formation: $6C(c) + 3H_2(g) = C_6H_6(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.520	64.340	64.340	0	19.820	31.005	-22.727
300	19.650	64.470	64.340	.040	19.797	31.074	-22.637
400	26.740	71.110	65.185	2.370	18.581	35.033	-19.141
500	32.800	77.750	67.030	5.360	17.572	39.267	-17.163
600	37.740	84.180	69.363	8.890	16.740	43.686	-15.912
700	41.750	90.310	71.924	12.870	16.070	48.227	-15.057
800	45.060	96.110	74.585	17.220	15.548	52.864	-14.442
900	47.830	101.580	77.291	21.860	15.133	57.539	-13.972
1000	50.160	106.740	79.970	26.770	14.847	62.277	-13.610

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 20.796 + 31.644x10^{-3}T - 9.521x10^{5}T^{-2}$
$H°- H°_{298} = 20.796x10^{-3}T + 15.822x10^{-6}T^{2} + 9.521x10^{2}T^{-1} - 10.800$

Formation equations (kcal/mol):

298.15-1000 K: $ΔHf° = 24.909 - 19.680x10^{-3}T + 9.969x10^{-6}T^{2} - 32.200T^{-1}$
$ΔGf° = 24.909 + 19.680x10^{-3}T\ln T - 9.969x10^{-6}T^{2} - 16.100T^{-1} - 88.532x10^{-3}T$

Source: Data from Stull (479).

CN(g)
Carbon Mononitride (ideal gas)
[Formation: C(c) + $0.5N_2(g)$ = CN(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	6.968	48.406	48.406	0	109.000	101.800	-74.620
300	6.969	48.449	48.406	.013	109.003	101.755	-74.128
400	7.029	50.460	48.680	.712	109.109	99.322	-54.266
500	7.155	52.041	49.199	1.421	109.149	96.869	-42.341
600	7.326	53.360	49.785	2.145	109.140	94.414	-34.390
700	7.510	54.503	50.380	2.886	109.093	91.962	-28.711
800	7.689	55.518	50.959	3.647	109.024	89.520	-24.455
900	7.852	56.433	51.517	4.424	108.935	87.086	-21.147
1000	7.996	57.268	52.052	5.216	108.832	84.663	-18.503
1100	8.123	58.036	52.561	6.022	108.720	82.262	-16.344
1200	8.235	58.748	53.048	6.840	108.600	79.851	-14.543
1300	8.337	59.411	53.512	7.669	108.473	77.461	-13.022
1400	8.431	60.033	53.956	8.508	108.343	75.080	-11.720
1500	8.522	60.617	54.380	9.355	108.208	72.709	-10.594
1600	8.612	61.170	54.787	10.212	108.072	70.348	-9.609
1700	8.702	61.695	55.179	11.078	107.935	67.993	-8.741
1800	8.794	62.195	55.555	11.952	107.798	65.647	-7.971
1900	8.890	62.673	55.917	12.837	107.664	63.310	-7.282
2000	8.989	63.131	56.266	13.730	107.531	60.979	-6.663

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 6.658 + 1.242\times10^{-3}T - 0.054\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.658\times10^{-3}T + 0.621\times10^{-6}T^{2} + 0.054\times10^{2}T^{-1} - 2.058$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 109.621 - 0.119\times10^{-3}T - 0.440\times10^{-6}T^{2} - 162.950T^{-1}$

$\Delta Gf^\circ = 109.621 + 0.119\times10^{-3}T\ln T + 0.440\times10^{-6}T^{2} - 81.475T^{-1} - 26.121\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (392). Other data from JANAF (127).

$C_2N_2(g)$
Dicarbon Dinitride (ideal gas), Cyanogen
[Formation: $2C(c) + N_2(g) = C_2N_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.563	57.711	57.711	0	73.870	71.128	-52.137
300	13.590	57.795	57.712	.025	73.874	71.110	-51.803
400	14.771	61.878	58.260	1.447	74.111	70.153	-38.330
500	15.615	65.269	59.333	2.968	74.295	69.141	-30.221
600	16.305	68.178	60.570	4.565	74.425	68.098	-24.804
700	16.899	70.737	61.843	6.226	74.511	67.036	-20.929
800	17.415	73.028	63.101	7.942	74.566	65.964	-18.020
900	17.858	75.106	64.320	9.707	74.598	64.885	-15.756
1000	18.237	77.007	65.495	11.512	74.614	63.805	-13.944
1100	18.559	78.761	66.623	13.352	74.618	62.745	-12.466
1200	18.833	80.388	67.703	15.222	74.612	61.644	-11.227
1300	19.066	81.905	68.738	17.117	74.596	60.564	-10.182
1400	19.264	83.325	69.729	19.034	74.574	59.485	-9.286
1500	19.434	84.660	70.681	20.969	74.544	58.409	-8.510
1600	19.579	85.919	71.594	22.920	74.511	57.335	-7.831
1700	19.705	87.110	72.472	24.885	74.469	56.260	-7.233
1800	19.815	88.240	73.317	26.861	74.423	55.192	-6.701
1900	19.910	89.314	74.131	28.847	74.372	54.124	-6.226
2000	19.993	90.337	74.916	30.842	74.313	53.061	-5.798

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 15.344 + 2.836 \times 10^{-3}T - 2.335 \times 10^{5}T^{-2}$

$H°- H°_{298} = 15.344 \times 10^{-3}T + 1.418 \times 10^{-6}T^{2} + 2.335 \times 10^{2}T^{-1} - 5.484$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 73.745 + 1.791 \times 10^{-3}T - 0.703 \times 10^{-6}T^{2} - 103.200T^{-1}$

$\Delta Gf° = 73.745 - 1.791 \times 10^{-3}T\ln T + 0.703 \times 10^{-6}T^{2} - 51.600T^{-1} + 1.799 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (392). Other data from JANAF (127).

$C_4N_2(g)$
Tetracarbon Dinitride (ideal gas)
[Formation: $4C(c) + N_2(g) = C_4N_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	20.528	69.314	69.314	0	127.500	122.117	-89.513
300	20.576	69.441	69.314	.038	127.509	122.083	-88.936
400	22.664	75.666	70.148	2.207	128.005	120.199	-65.673
500	24.162	80.892	71.788	4.552	128.379	118.200	-51.665
600	25.370	85.407	73.690	7.030	128.636	116.140	-42.304
700	26.391	89.397	75.656	9.619	128.802	114.041	-35.605
800	27.259	92.979	77.600	12.303	128.907	111.927	-30.577
900	27.996	96.233	79.492	15.067	128.964	109.797	-26.662
1000	28.617	99.216	81.318	17.898	128.992	107.664	-23.530
1100	29.141	101.969	83.072	20.787	128.997	105.574	-20.975
1200	29.582	104.524	84.754	23.724	128.982	103.402	-18.832
1300	29.955	106.907	86.368	26.701	128.948	101.271	-17.025
1400	30.272	109.139	87.915	29.713	128.903	99.142	-15.477
1500	30.542	111.237	89.401	32.754	128.843	97.019	-14.135
1600	30.773	113.215	90.827	35.820	128.777	94.903	-12.963
1700	30.972	115.087	92.200	38.908	128.694	92.783	-11.928
1800	31.145	116.863	93.522	42.014	128.604	90.676	-11.009
1900	31.295	118.551	94.795	45.136	128.505	88.571	-10.188
2000	31.426	120.159	96.023	48.272	128.391	86.475	-9.449
2100	31.541	121.695	97.209	51.420	128.269	84.375	-8.781
2200	31.642	123.165	98.356	54.580	128.140	82.290	-8.175
2300	31.732	124.574	99.466	57.749	128.001	80.216	-7.622
2400	31.813	125.926	100.540	60.926	127.847	78.136	-7.115
2500	31.884	127.226	101.582	64.111	127.690	76.068	-6.650

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 24.770 + 3.726\times10^{-3}T - 4.758\times10^{5}T^{-2}$

$H°- H°_{298} = 24.770\times10^{-3}T + 1.863\times10^{-6}T^{2} + 4.758\times10^{2}T^{-1} - 9.147$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 127.102 + 4.181\times10^{-3}T - 1.790\times10^{-6}T^{2} - 205.500T^{-1}$

$\Delta Gf° = 127.102 - 4.181\times10^{-3}T\ln T + 1.790\times10^{-6}T^{2} - 102.750T^{-1} + 7.723\times10^{-3}T$

2000-2500 K: $\Delta Hf° = 137.743 - 6.439\times10^{-3}T + 1.271\times10^{-6}T^{2} - 3496.200T^{-1}$

$\Delta Gf° = 137.743 + 6.439\times10^{-3}T\ln T - 1.271\times10^{-6}T^{2} - 1748.100T^{-1} - 71.786\times10^{-3}T$

Source: Data from JANAF (127).

$CNBr(g)$
Cyanogen Bromide (ideal gas)
[Formation: $C(c) + 0.5N_2(g) + 0.5Br_2(l,g) = CNBr(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.263	59.334	59.334	0	44.500	39.465	-28.928
300	11.280	59.404	59.334	.021	44.494	39.434	-28.727
332.6	11.509	60.579	59.399	.392	44.387	38.889	-25.554
332.6	11.509	60.579	59.399	.392	40.854	38.889	-25.554
400	11.983	62.751	59.786	1.186	40.945	38.481	-21.025
500	12.451	65.477	60.661	2.408	41.058	37.851	-16.544
600	12.826	67.781	61.659	3.673	41.146	37.202	-13.551
700	13.150	69.783	62.680	4.972	41.210	36.539	-11.408
800	13.433	71.557	63.681	6.301	41.261	35.869	-9.799
900	13.680	73.154	64.646	7.657	41.302	35.191	-8.545
1000	13.895	74.607	65.571	9.036	41.336	34.509	-7.542
1100	14.081	75.940	66.454	10.435	41.366	33.836	-6.722
1200	14.244	77.173	67.296	11.852	41.394	33.139	-6.035
1300	14.386	78.318	68.100	13.283	41.417	32.451	-5.455
1400	14.511	79.389	68.869	14.728	41.439	31.760	-4.958
1500	14.621	80.394	69.604	16.185	41.460	31.068	-4.527
1600	14.720	81.341	70.309	17.652	41.480	30.375	-4.149
1700	14.809	82.236	70.984	19.129	41.499	29.679	-3.815
1800	14.890	83.085	71.633	20.614	41.517	28.985	-3.519
1900	14.965	83.892	72.257	22.106	41.535	28.288	-3.254
2000	15.033	84.661	72.858	23.606	41.551	27.590	-3.015

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.251 + 1.638\times10^{-3}T - 1.313\times10^{5}T^{-2}$

$H°-H°_{298} = 12.251\times10^{-3}T + 0.819\times10^{-6}T^2 + 1.313\times10^{2}T^{-1} - 4.166$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = 45.706 - 3.571\times10^{-3}T - 0.191\times10^{-6}T^2 - 37.050T^{-1}$

$\Delta Gf° = 45.706 + 3.571\times10^{-3}T\ln T + 0.191\times10^{-6}T^2 - 18.525T^{-1} - 41.127\times10^{-3}T$

332.6-2000 K: $\Delta Hf° = 40.706 + 1.010\times10^{-3}T - 0.269\times10^{-6}T^2 - 52.750T^{-1}$

$\Delta Gf° = 40.706 - 1.010\times10^{-3}T\ln T + 0.269\times10^{-6}T^2 - 26.375T^{-1} + 0.550\times10^{-3}T$

Source: Data from JANAF (127).

$CNCl(g)$
Cyanogen Chloride (ideal gas)
[Formation: $C(c) + 0.5N_2(g) + 0.5Cl_2(g) = CNCl(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.820	56.459	56.459	0	32.970	31.313	-22.953
300	10.838	56.526	56.459	.020	32.972	31.303	-22.804
400	11.644	59.760	56.895	1.146	33.090	30.728	-16.789
500	12.195	62.420	57.742	2.339	33.189	30.126	-13.168
600	12.627	64.683	58.715	3.581	33.263	29.507	-10.748
700	12.991	66.657	59.711	4.862	33.317	28.876	-9.015
800	13.302	68.413	60.692	6.177	33.359	28.238	-7.714
900	13.571	69.995	61.638	7.521	33.391	27.595	-6.701
1000	13.802	71.437	62.547	8.890	33.418	26.950	-5.890
1100	13.983	72.761	63.416	10.279	33.441	26.312	-5.228
1200	14.150	73.985	64.247	11.686	33.460	25.652	-4.672
1300	14.304	75.124	65.040	13.109	33.477	25.001	-4.203
1400	14.444	76.189	65.799	14.546	33.492	24.348	-3.801
1500	14.570	77.190	66.525	15.997	33.508	23.695	-3.452
1600	14.667	78.134	67.222	17.459	33.524	23.040	-3.147
1700	14.757	79.026	67.891	18.930	33.537	22.383	-2.877
1800	14.843	79.872	68.533	20.410	33.550	21.727	-2.638
1900	14.923	80.676	69.150	21.899	33.565	21.072	-2.424
2000	14.997	81.444	69.746	23.395	33.576	20.413	-2.231

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.076 + 1.722\times10^{-3}T - 1.573\times10^{5}T^{-2}$

$H°- H°_{298} = 12.076\times10^{-3}T + 0.861\times10^{-6}T^{2} + 1.573\times10^{2}T^{-1} - 4.205$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 32.879 + 0.886\times10^{-3}T - 0.244\times10^{-6}T^{2} - 45.200T^{-1}$

$\Delta Gf° = 32.879 - 0.886\times10^{-3}T\ln T + 0.244\times10^{-6}T^{2} - 22.600T^{-1} - 0.022\times10^{-3}T$

Source: Data from JANAF (127).

CNF(g)
Cyanogen Fluoride (ideal gas)
[Formation: $C(c) + 0.5N_2(g) + 0.5F_2(g) = CNF(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.113	53.846	53.846	0	8.600	7.000	-5.131
300	10.130	53.908	53.846	.019	8.602	6.990	-5.092
400	10.934	56.939	54.254	1.074	8.680	6.441	-3.519
500	11.542	59.447	55.049	2.199	8.734	5.874	-2.567
600	12.031	61.596	55.964	3.379	8.766	5.299	-1.930
700	12.438	63.482	56.906	4.603	8.778	4.720	-1.474
800	12.779	65.166	57.836	5.864	8.778	4.140	-1.131
900	13.066	66.688	58.736	7.157	8.769	3.561	-.865
1000	13.306	68.077	59.601	8.476	8.753	2.982	-.652
1100	13.508	69.355	60.430	9.817	8.733	2.417	-.480
1200	13.677	70.538	61.225	11.176	8.709	1.832	-.334
1300	13.820	71.639	61.984	12.551	8.681	1.261	-.212
1400	13.942	72.668	62.711	13.940	8.650	.690	-.108
1500	14.045	73.633	63.407	15.339	8.615	.123	-.018
1600	14.133	74.542	64.075	16.748	8.579	-.440	.060
1700	14.210	75.402	64.717	18.165	8.538	-1.005	.129
1800	14.275	76.216	65.333	19.590	8.497	-1.564	.190
1900	14.333	76.989	65.926	21.020	8.451	-2.121	.244
2000	14.383	77.726	66.498	22.456	8.402	-2.677	.293

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.355 + 1.896\text{x}10^{-3}T - 1.606\text{x}10^{5}T^{-2}$

$H°-H°_{298} = 11.355\text{x}10^{-3}T + 0.948\text{x}10^{-6}T^{2} + 1.606\text{x}10^{2}T^{-1} - 4.008$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 8.716 + 0.324\text{x}10^{-3}T - 0.200\text{x}10^{-6}T^{2} - 58.000T^{-1}$

$\Delta Gf° = 8.716 - 0.324\text{x}10^{-3}T\ln T + 0.200\text{x}10^{-6}T^{2} - 29.000T^{-1} - 3.639\text{x}10^{-3}T$

Source: Data from JANAF (127).

CNI(g)
Cyanogen Iodide (ideal gas)
[Formation: $C(c) + 0.5N_2(g) + 0.5I_2(c,l,g) = CNI(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.573	61.479	61.479	0	54.000	47.040	-34.481
300	11.587	61.550	61.480	.021	53.999	46.997	-34.237
386.8	12.077	64.562	61.845	1.051	53.915	44.980	-25.415
386.8	12.077	64.562	61.845	1.051	52.060	44.980	-25.415
400	12.152	64.969	61.942	1.211	52.010	44.740	-24.444
458.4	12.369	66.641	62.434	1.928	51.783	43.695	-20.832
458.4	12.369	66.641	62.434	1.928	46.772	43.695	-20.832
500	12.523	67.722	62.830	2.446	46.818	43.415	-18.976
600	12.825	70.033	63.845	3.713	46.903	42.725	-15.562
700	13.090	72.030	64.874	5.009	46.961	42.023	-13.120
800	13.323	73.794	65.882	6.330	47.002	41.316	-11.287
900	13.524	75.375	66.849	7.673	47.026	40.602	-9.859
1000	13.698	76.809	67.775	9.034	47.040	39.888	-8.717
1100	13.845	78.122	68.657	10.412	47.047	39.183	-7.785
1200	13.971	79.332	69.496	11.803	47.045	38.457	-7.004
1300	14.078	80.454	70.296	13.205	47.037	37.743	-6.345
1400	14.169	81.501	71.060	14.618	47.025	37.028	-5.780
1500	14.247	82.481	71.788	16.039	47.007	36.315	-5.291
1600	14.314	83.403	72.486	17.467	46.986	35.603	-4.863
1700	14.372	84.273	73.155	18.901	46.958	34.890	-4.485
1800	14.422	85.096	73.795	20.341	46.929	34.182	-4.150
1900	14.466	85.877	74.411	21.785	46.895	33.474	-3.850
2000	14.504	86.619	75.002	23.234	46.857	32.771	-3.581

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:

$$Cp° = 12.402 + 1.280\times10^{-3}T - 1.076\times10^{5}T^{-2}$$

$$H°-H°_{298} = 12.402\times10^{-3}T + 0.640\times10^{-6}T^{2} + 1.076\times10^{2}T^{-1} - 4.115$$

Formation equations (kcal/mol):

298.15-386.8 K:

$$\Delta Hf° = 54.550 - 0.813\times10^{-3}T - 1.167\times10^{-6}T^{2} - 60.750T^{-1}$$

$$\Delta Gf° = 54.550 + 0.813\times10^{-3}T\ln T + 1.167\times10^{-6}T^{2} - 30.375T^{-1} - 29.825\times10^{-3}T$$

386.8-458.4 K:

$$\Delta Hf° = 53.822 - 4.015\times10^{-3}T - 0.421\times10^{-6}T^{2} - 60.750T^{-1}$$

$$\Delta Gf° = 53.822 + 4.015\times10^{-3}T\ln T + 0.421\times10^{-6}T^{2} - 30.375T^{-1} - 46.733\times10^{-3}T$$

458.4-2000 K:

$$\Delta Hf° = 46.466 + 1.155\times10^{-3}T - 0.455\times10^{-6}T^{2} - 68.400T^{-1}$$

$$\Delta Gf° = 46.466 - 1.155\times10^{-3}T\ln T + 0.455\times10^{-6}T^{2} - 34.200T^{-1} + 0.998\times10^{-3}T$$

Source: Data from JANAF (127).

$COCl_2(g)$
Carbonyl Dichloride (ideal gas)
[Formation: $C(c) + 0.5O_2(g) + Cl_2(g) = COCl_2(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	13.790	67.816	67.816	0	-52.600	-49.216	36.076
300	13.823	67.901	67.816	.026	-52.599	-49.195	35.838
400	15.282	72.092	68.377	1.486	-52.568	-48.064	26.261
500	16.269	75.615	69.483	3.066	-52.524	-46.943	20.519
600	16.981	78.647	70.762	4.731	-52.482	-45.829	16.693
700	17.515	81.307	72.083	6.457	-52.447	-44.724	13.963
800	17.924	83.674	73.387	8.230	-52.418	-43.624	11.917
900	18.242	85.804	74.650	10.039	-52.394	-42.526	10.327
1000	18.493	87.739	75.863	11.876	-52.371	-41.432	9.055
1100	18.693	89.512	77.025	13.736	-52.351	-40.328	8.012
1200	18.855	91.145	78.134	15.613	-52.337	-39.247	7.148
1300	18.986	92.660	79.195	17.505	-52.325	-38.158	6.415
1400	19.095	94.071	80.207	19.410	-52.314	-37.068	5.786
1500	19.186	95.392	81.176	21.324	-52.310	-35.980	5.242
1600	19.262	96.632	82.103	23.246	-52.308	-34.890	4.766
1700	19.326	97.802	82.993	25.176	-52.310	-33.800	4.345
1800	19.381	98.908	83.846	27.111	-52.317	-32.711	3.972
1900	19.428	99.957	84.666	29.052	-52.327	-31.620	3.637
2000	19.469	100.955	85.457	30.997	-52.345	-30.531	3.336

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.806 + 1.746x10^{-3}T - 3.144x10^{5}T^{-2}$

$H°-H°_{298} = 16.806x10^{-3}T + 0.873x10^{-6}T^{2} + 3.144x10^{2}T^{-1} - 6.143$

Formation equations (kcal/mol):

298.15-2000 K: $ΔHf° = -53.003 + 0.846x10^{-3}T - 0.232x10^{-6}T^{2} + 51.200T^{-1}$

$ΔGf° = -53.003 - 0.846x10^{-3}TlnT + 0.232x10^{-6}T^{2} + 25.600T^{-1} + 17.164x10^{-3}T$

Source: Data from JANAF (127).

$COF_2(g)$
Carbonyl Difluoride (ideal gas)
[Formation: $C(c) + 0.5O_2(g) + F_2(g) = COF_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.294	61.851	61.851	0	-152.700	-148.983	109.206
300	11.330	61.921	61.851	.021	-152.704	-148.960	108.516
400	13.092	65.432	62.319	1.245	-152.848	-147.689	80.693
500	14.460	68.507	63.255	2.626	-152.953	-146.386	63.985
600	15.505	71.240	64.362	4.127	-153.036	-145.064	52.839
700	16.306	73.693	65.523	5.719	-153.105	-143.730	44.874
800	16.924	75.912	66.685	7.382	-153.162	-142.387	38.898
900	17.406	77.935	67.825	9.099	-153.210	-141.038	34.248
1000	17.786	79.789	68.929	10.860	-153.250	-139.684	30.528
1100	18.089	81.499	69.995	12.654	-153.285	-138.314	27.480
1200	18.344	83.084	71.021	14.475	-153.317	-136.964	24.944
1300	18.533	84.559	72.006	16.319	-153.346	-135.598	22.796
1400	18.697	85.939	72.953	18.181	-153.376	-134.234	20.955
1500	18.834	87.234	73.862	20.058	-153.404	-132.866	19.358
1600	18.949	88.453	74.736	21.947	-153.434	-131.494	17.961
1700	19.046	89.605	75.577	23.847	-153.465	-130.122	16.728
1800	19.129	90.696	76.387	25.756	-153.499	-128.747	15.632
1900	19.201	91.732	77.168	27.672	-153.535	-127.371	14.651
2000	19.262	92.719	77.921	29.596	-153.576	-125.993	13.768

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.853 + 2.886\times10^{-3}T - 3.929\times10^{5}T^{-2}$

$H°-H°_{298} = 14.853\times10^{-3}T + 1.443\times10^{-6}T^{2} + 3.929\times10^{2}T^{-1} - 5.874$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -152.814 - 0.788\times10^{-3}T + 0.252\times10^{-6}T^{2} + 97.500T^{-1}$

$\Delta Gf° = -152.814 + 0.788\times10^{-3}T\ln T - 0.252\times10^{-6}T^{2} + 48.750T^{-1} + 7.887\times10^{-3}T$

Source: Data from JANAF (127).

$CSe(g)$
Carbon Monoselenide (ideal gas)
[Reaction: $C(c) + 0.5Se_2(g) = CSe(g)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	7.010	53.200	53.200	0	71.050	64.274	-47.113
300	7.010	53.240	53.200	.013	71.050	64.232	-46.793
400	7.290	55.310	53.485	.730	71.026	61.959	-33.852
500	7.470	56.950	54.014	1.468	70.942	59.703	-26.096
600	7.620	58.330	54.625	2.223	70.815	57.464	-20.931
700	7.750	59.510	55.237	2.991	70.654	55.255	-17.251
800	7.870	60.550	55.835	3.772	70.472	53.071	-14.498
900	7.980	61.490	56.419	4.564	70.275	50.899	-12.360
1000	8.100	62.330	56.962	5.368	70.073	48.763	-10.657
1100	8.210	63.110	57.489	6.183	69.866	46.650	-9.268
1200	8.310	63.830	57.989	7.009	69.660	44.536	-8.111
1300	8.420	64.500	58.465	7.846	69.456	42.452	-7.137
1400	8.530	65.130	58.921	8.693	69.256	40.376	-6.303
1500	8.630	65.720	59.353	9.551	69.060	38.323	-5.584
1600	8.740	66.280	59.767	10.420	68.872	36.280	-4.956
1700	8.850	66.810	60.164	11.299	68.690	34.260	-4.404
1800	8.950	67.320	60.548	12.189	68.517	32.234	-3.914
1900	9.060	67.810	60.921	13.090	68.352	30.215	-3.475
2000	9.160	68.280	61.279	14.001	68.195	28.205	-3.082

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.089 + 1.040\text{x}10^{-3}T - 0.346\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.089\text{x}10^{-3}T + 0.520\text{x}10^{-6}T^{2} + 0.346\text{x}10^{2}T^{-1} - 2.276$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = 72.145 - 1.761\text{x}10^{-3}T - 0.086\text{x}10^{-6}T^{2} - 167.650T^{-1}$

$\Delta Gr^\circ = 72.145 + 1.761\text{x}10^{-3}T\ln T + 0.086\text{x}10^{-6}T^{2} - 83.825T^{-1} - 35.517\text{x}10^{-3}T$

Source: Data from Mills (332).

$CSe_2(g)$
Carbon Diselenide (ideal gas)
[Reaction: $C(c) + Se_2(g) = CSe_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hr°$	$\Delta Gr°$	
298.15	11.960	62.900	62.900	0	28.400	27.408	-20.090
300	11.990	62.970	62.900	.022	28.400	27.402	-19.962
400	12.860	66.560	63.380	1.272	28.411	27.068	-14.789
500	13.310	69.490	64.326	2.582	28.396	26.729	-11.683
600	13.580	71.940	65.395	3.927	28.353	26.399	-9.616
700	13.770	74.050	66.486	5.295	28.287	26.079	-8.142
800	13.920	75.900	67.550	6.680	28.205	25.772	-7.041
900	14.050	77.540	68.563	8.079	28.113	25.477	-6.187
1000	14.150	79.030	69.541	9.489	28.017	25.182	-5.503
1100	14.250	80.380	70.463	10.909	27.919	24.920	-4.951
1200	14.340	81.630	71.347	12.339	27.823	24.635	-4.487
1300	14.430	82.780	72.182	13.778	27.729	24.379	-4.098
1400	14.520	83.850	72.975	15.225	27.640	24.122	-3.766
1500	14.600	84.860	73.739	16.681	27.557	23.865	-3.477
1600	14.680	85.800	74.460	18.144	27.481	23.625	-3.227
1700	14.750	86.690	75.151	19.616	27.412	23.403	-3.009
1800	14.830	87.540	75.821	21.095	27.351	23.153	-2.811
1900	14.900	88.340	76.455	22.581	27.298	22.924	-2.637
2000	14.980	89.110	77.072	24.076	27.255	22.685	-2.479

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.625 + 0.698\times10^{-3}T - 1.665\times10^{5}T^{-2}$

$H°-H°_{298} = 13.625\times10^{-3}T + 0.349\times10^{-6}T^{2} + 1.665\times10^{2}T^{-1} - 4.652$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = 28.795 - 0.557\times10^{-3}T - 0.098\times10^{-6}T^{2} - 65.700T^{-1}$

$\Delta Gr° = 28.795 + 0.557\times10^{-3}T\ln T + 0.098\times10^{-6}T^{2} - 32.850T^{-1} - 7.487\times10^{-3}T$

Source: Data from Mills (332).

$CaAl_2O_4(c)$
Calcium Aluminate
[Formation: $Ca(c,l,g) + 2Al(c,l) + 2O_2(g) = CaAl_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.830	27.300	27.300	0	-556.000	-527.914	386.966
300	28.948	27.479	27.302	.053	-556.006	-527.739	384.453
400	33.318	36.478	28.498	3.192	-556.099	-518.294	283.179
500	35.710	44.191	30.885	6.653	-555.991	-508.853	222.417
600	37.315	50.851	33.669	10.309	-555.831	-499.435	181.917
700	38.546	56.699	36.550	14.104	-555.688	-490.052	152.999
720	38.751	57.788	37.125	14.877	-555.667	-488.174	148.179
720	38.751	57.788	37.125	14.877	-555.887	-488.174	148.179
800	39.572	61.915	39.401	18.011	-555.781	-480.657	131.308
900	40.473	66.629	42.169	22.014	-555.736	-471.256	114.435
933.61	40.747	68.118	43.077	23.379	-555.755	-468.101	109.577
933.61	40.747	68.118	43.077	23.379	-560.915	-468.101	109.577
1000	41.287	70.936	44.833	26.103	-560.949	-461.517	100.863
1100	42.036	74.907	47.390	30.269	-561.006	-451.570	89.718
1112	42.119	75.364	47.689	30.774	-561.016	-450.382	88.516
1112	42.119	75.364	47.689	30.774	-563.056	-450.382	88.516
1200	42.729	78.595	49.838	34.508	-562.767	-441.475	80.402
1300	43.372	82.040	52.183	38.814	-562.391	-431.382	72.521
1400	43.966	85.277	54.433	43.181	-561.970	-421.319	65.770
1500	44.511	88.329	56.592	47.605	-561.504	-411.295	59.925
1600	45.004	91.218	58.667	52.081	-561.000	-401.301	54.814
1700	45.445	93.959	60.663	56.604	-560.459	-391.324	50.308
1757	45.664	95.462	61.768	59.201	-560.137	-385.659	47.971
1757	45.664	95.462	61.768	59.201	-596.763	-385.659	47.971
1800	45.829	96.568	62.586	61.168	-596.429	-380.463	46.194

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 35.891 + 6.048\times10^{-3}T - 7.879\times10^{5}T^{-2}$
$H°- H°_{298} = 35.891\times10^{-3}T + 3.024\times10^{-6}T^{2} + 7.879\times10^{2}T^{-1} - 13.612$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -560.814 + 8.416\times10^{-3}T - 4.006\times10^{-6}T^{2} + 793.300T^{-1}$
$\Delta Gf° = -560.814 - 8.416\times10^{-3}T\ln T + 4.006\times10^{-6}T^{2} + 396.650T^{-1} + 152.642\times10^{-3}T$
720-933.61 K: $\Delta Hf° = -562.555 + 12.354\times10^{-3}T - 6.378\times10^{-6}T^{2} + 732.300T^{-1}$
$\Delta Gf° = -562.555 - 12.354\times10^{-3}T\ln T + 6.378\times10^{-6}T^{2} + 366.150T^{-1} + 179.320\times10^{-3}T$
933.61-1112 K: $\Delta Hf° = -565.090 + 6.358\times10^{-3}T - 2.924\times10^{-6}T^{2} + 697.500T^{-1}$
$\Delta Gf° = -565.090 - 6.358\times10^{-3}T\ln T + 2.924\times10^{-6}T^{2} + 348.750T^{-1} + 144.274\times10^{-3}T$
1112-1757 K: $\Delta Hf° = -565.338 - 0.749\times10^{-3}T + 2.018\times10^{-6}T^{2} + 697.500T^{-1}$
$\Delta Gf° = -565.338 + 0.749\times10^{-3}T\ln T - 2.018\times10^{-6}T^{2} + 348.750T^{-1} + 100.145\times10^{-3}T$
1757-1800 K: $\Delta Hf° = -605.509 + 1.281\times10^{-3}T + 2.011\times10^{-6}T^{2} + 697.500T^{-1}$
$\Delta Gf° = -605.509 - 1.281\times10^{-3}T\ln T - 2.011\times10^{-6}T^{2} + 348.750T^{-1} + 138.163\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Koehler (276). Low-temperature heat capacities and entropy at 298 K from King (261). High-temperature data based on Bonnickson (53).

$CaAl_4O_7(c)$
Calcium Dialuminate
[Formation: $Ca(c,l,g) + 4Al(c,l) + 3.5O_2(g) = CaAl_4O_7(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	47.700	42.500	42.500	0	-951.000	-901.489	660.801
300	47.924	42.796	42.503	.088	-951.013	-901.181	656.502
400	56.443	57.903	44.503	5.360	-951.234	-884.521	483.273
500	61.140	71.044	48.530	11.257	-951.034	-867.860	379.337
600	64.260	82.483	53.255	17.537	-950.685	-851.249	310.063
700	66.545	92.568	58.165	24.082	-950.323	-834.709	260.605
720	66.897	94.448	59.147	25.416	-950.258	-831.404	252.362
720	66.897	94.448	59.147	25.416	-950.478	-831.404	252.362
800	68.306	101.574	63.039	30.828	-950.211	-818.191	223.516
900	69.692	109.703	67.780	37.731	-950.008	-801.688	194.674
933.61	70.058	112.265	69.335	40.079	-949.988	-796.149	186.369
933.61	70.058	112.265	69.335	40.079	-960.308	-796.149	186.369
1000	70.781	117.104	72.347	44.757	-960.224	-784.497	171.449
1100	71.616	123.891	76.728	51.879	-960.102	-766.928	152.373
1112	71.689	124.668	77.241	52.739	-960.091	-764.826	150.315
1112	71.689	124.668	77.241	52.739	-962.131	-764.826	150.315
1200	72.225	130.150	80.923	59.072	-961.698	-749.226	136.451
1300	72.624	135.949	84.936	66.317	-961.185	-731.545	122.982
1400	72.824	141.339	88.774	73.591	-960.672	-713.896	111.443
1500	72.834	146.365	92.448	80.875	-960.169	-696.297	101.449
1600	72.657	151.061	95.967	88.151	-959.698	-678.723	92.708
1700	72.299	155.456	99.338	95.400	-959.272	-661.165	84.997
1757	71.992	157.836	101.197	99.514	-959.056	-651.170	80.997
1757	71.992	157.836	101.197	99.514	-995.682	-651.170	80.997
1800	71.761	159.574	102.571	102.605	-995.451	-642.709	78.034

Phase changes: 720 K, α - β transition point of Ca; $\Delta H^\circ = 0.220$ kcal/mol.
933.61 K, melting point of Al; $\Delta H^\circ = 2.580$ kcal/mol.
1112 K, melting point of Ca; $\Delta H^\circ = 2.040$ kcal/mol.
1757 K, boiling point of Ca; $\Delta H^\circ = 36.626$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $C_p^\circ = 66.526 + 5.100\times10^{-3}T - 18.087\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 66.526\times10^{-3}T + 2.550\times10^{-6}T^2 + 18.087\times10^{2}T^{-1} - 26.128$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -961.873 + 19.022\times10^{-3}T - 8.689\times10^{-6}T^2 + 1781.100T^{-1}$
$\Delta Gf^\circ = -961.873 - 19.022\times10^{-3}T\ln T + 8.689\times10^{-6}T^2 + 890.550T^{-1} + 298.300\times10^{-3}T$
720-933.61 K: $\Delta Hf^\circ = -963.614 + 22.960\times10^{-3}T - 11.061\times10^{-6}T^2 + 1720.100T^{-1}$
$\Delta Gf^\circ = -963.614 - 22.960\times10^{-3}T\ln T + 11.061\times10^{-6}T^2 + 860.050T^{-1} + 324.978\times10^{-3}T$
933.61-1112 K: $\Delta Hf^\circ = -968.685 + 10.968\times10^{-3}T - 4.153\times10^{-6}T^2 + 1650.500T^{-1}$
$\Delta Gf^\circ = -968.685 - 10.968\times10^{-3}T\ln T + 4.153\times10^{-6}T^2 + 825.250T^{-1} + 254.885\times10^{-3}T$
1112-1757 K: $\Delta Hf^\circ = -968.933 + 3.861\times10^{-3}T + 0.790\times10^{-6}T^2 + 1650.500T^{-1}$
$\Delta Gf^\circ = -968.933 - 3.861\times10^{-3}T\ln T - 0.790\times10^{-6}T^2 + 825.250T^{-1} + 210.756\times10^{-3}T$
1757-1800 K: $\Delta Hf^\circ = -1009.104 + 5.891\times10^{-3}T + 0.783\times10^{-6}T^2 + 1650.500T^{-1}$
$\Delta Gf^\circ = -1009.104 - 5.891\times10^{-3}T\ln T - 0.783\times10^{-6}T^2 + 825.250T^{-1} + 248.774\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Koehler (276). Low-temperature heat capacities and entropy at 298 K from King (261). High-temperature data based on Bonnickson (53).

$Ca_3Al_2O_6(c)$
Tricalcium Aluminate
[Formation: $3Ca(c,l,g) + 2Al(c,l) + 3O_2(g) = Ca_3Al_2O_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	50.140	49.200	49.200	0	-857.500	-815.405	597.700
300	50.301	49.511	49.201	.093	-857.501	-815.141	593.822
400	56.367	64.934	51.264	5.468	-857.300	-801.042	437.663
500	59.550	77.884	55.328	11.278	-856.860	-787.028	344.005
600	61.599	88.934	60.032	17.341	-856.416	-773.096	281.596
700	63.080	98.546	64.862	23.579	-856.072	-759.252	237.046
720	63.310	100.326	65.822	24.843	-856.026	-756.475	229.619
720	63.310	100.326	65.822	24.843	-856.686	-756.475	229.619
800	64.228	107.047	69.615	29.946	-856.435	-745.353	203.618
900	65.157	114.667	74.204	36.417	-856.356	-731.429	177.613
933.61	65.415	117.061	75.704	38.611	-856.425	-726.762	170.126
933.61	65.415	117.061	75.704	38.611	-861.585	-726.762	170.126
1000	65.926	121.573	78.600	42.973	-861.825	-717.220	156.746
1100	66.568	127.888	82.799	49.598	-862.316	-702.732	139.618
1112	66.632	128.611	83.289	50.397	-862.393	-701.007	137.772
1112	66.632	128.611	83.289	50.397	-868.513	-701.007	137.772
1200	67.104	133.704	86.801	56.283	-868.051	-687.768	125.258
1300	67.547	139.093	90.619	63.016	-867.504	-672.769	113.101
1400	67.904	144.112	94.263	69.789	-866.941	-657.805	102.687
1500	68.182	148.807	97.744	76.594	-866.364	-642.903	93.670
1600	68.384	153.214	101.075	83.423	-865.784	-628.032	85.784
1700	68.515	157.364	104.265	90.269	-865.202	-613.160	78.826
1757	68.549	159.625	106.025	94.176	-864.874	-604.717	75.219
1757	68.549	159.625	106.025	94.176	-974.752	-604.717	75.219
1800	68.574	161.283	107.325	97.124	-974.249	-595.569	72.311

Phase changes:
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 62.551 + 4.244x10^{-3}T - 12.157x10^{5}T^{-2}$
$H°- H^\circ_{298} = 62.551x10^{-3}T + 2.122x10^{-6}T^2 + 12.157x10^{2}T^{-1} - 22.916$

Formation equations (kcal/mol):

298.15-720 K: $ΔHf° = -866.933 + 20.184x10^{-3}T - 10.551x10^{-6}T^2 + 1297.900T^{-1}$
$ΔGf° = -866.933 - 20.184x10^{-3}TlnT + 10.551x10^{-6}T^2 + 648.950T^{-1} + 277.380x10^{-3}T$
720-933.61 K: $ΔHf° = -872.156 + 31.998x10^{-3}T - 17.667x10^{-6}T^2 + 1114.900T^{-1}$
$ΔGf° = -872.156 - 31.998x10^{-3}TlnT + 17.667x10^{-6}T^2 + 557.450T^{-1} + 357.415x10^{-3}T$
933.61-1112 K: $ΔHf° = -874.692 + 26.002x10^{-3}T - 14.213x10^{-6}T^2 + 1080.100T^{-1}$
$ΔGf° = -874.692 - 26.002x10^{-3}TlnT + 14.213x10^{-6}T^2 + 540.050T^{-1} + 322.368x10^{-3}T$
1112-1757 K: $ΔHf° = -875.436 + 4.681x10^{-3}T + 0.613x10^{-6}T^2 + 1080.100T^{-1}$
$ΔGf° = -875.436 - 4.681x10^{-3}TlnT - 0.613x10^{-6}T^2 + 540.050T^{-1} + 189.979x10^{-3}T$
1757-1800 K: $ΔHf° = -995.949 + 10.771x10^{-3}T + 0.592x10^{-6}T^2 + 1080.100T^{-1}$
$ΔGf° = -995.949 - 10.771x10^{-3}TlnT - 0.592x10^{-6}T^2 + 540.050T^{-1} + 304.034x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Koehler (276). Low-temperature heat capacities and entropy at 298 K from King (261). High-temperature data based on Bonnickson (53).

$Ca_{12}Al_{14}O_{33}$(c)
Calcium Aluminate
[Formation: $12Ca(c,l) + 14Al(c,l) + 16.5O_2(g) = Ca_{12}Al_{14}O_{33}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	259.200	250.200	250.200	0	-4644.000	-4413.671	3235.267
300	260	251.810	250.210	.480	-4644.021	-4412.233	3214.268
400	292.900	331.330	260.830	28.200	-4643.779	-4334.949	2368.476
500	315.300	399.260	281.880	58.690	-4641.803	-4257.951	1861.125
600	329.800	458.130	306.463	91.000	-4639.272	-4181.370	1523.043
700	339.100	509.720	331.891	124.480	-4636.961	-4105.299	1281.716
720	340.300	519.290	336.965	131.274	-4636.594	-4090.068	1241.489
720	340.300	519.290	336.965	131.274	-4639.234	-4090.068	1241.489
800	345.100	555.420	357.033	158.710	-4637.557	-4029.141	1100.696
900	350	596.350	381.394	193.460	-4636.598	-3952.985	959.904
933.61	351.882	609.217	389.366	205.255	-4636.689	-3927.452	919.370
933.61	351.882	609.217	389.366	205.255	-4672.809	-3927.452	919.370
1000	355.600	633.500	404.770	228.730	-4673.249	-3874.648	846.793
1100	364.000	667.760	427.142	264.680	-4674.092	-3794.727	753.933
1112	365.572	671.718	429.760	269.057	-4674.222	-3785.198	743.924
1112	365.572	671.718	429.760	269.057	-4698.702	-3785.198	743.924
1200	377.100	699.950	448.542	301.690	-4695.133	-3713.024	676.225
1300	396.700	730.860	469.075	340.320	-4689.653	-3631.408	610.487
1310	399.100	733.910	471.086	344.300	-4688.995	-3623.270	604.469
1310	357.300	733.910	471.086	344.300	-4688.995	-3623.270	604.469
1400	366.800	757.970	488.770	376.880	-4686.375	-3550.125	554.192
1500	377.400	783.630	507.563	414.100	-4682.536	-3469.143	505.447
1600	388.000	808.330	525.599	452.370	-4677.762	-3388.438	462.833
1700	398.600	832.170	542.935	491.700	-4672.011	-3307.905	425.255

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1310 K, second order transition of $Ca_{12}Al_{14}O_{33}$; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1310 K: $Cp° = 303.113 + 64.042\times10^{-3}T - 56.010\times10^{5}T^{-2}$
$H°-H°_{298} = 303.113\times10^{-3}T + 32.021\times10^{-6}T^{2} + 56.010\times10^{2}T^{-1} - 112.005$
1310-1700 K: $Cp° = 218.485 + 105.948\times10^{-3}T$
$H°-H°_{298} = 218.485\times10^{-3}T + 52.974\times10^{-6}T^{2} - 32.824$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -4682.706 + 73.558\times10^{-3}T - 31.296\times10^{-6}T^{2} + 5830.800T^{-1}$
$\Delta Gf° = -4682.706 - 73.558\times10^{-3}T\ln T + 31.296\times10^{-6}T^{2} + 2915.400T^{-1} + 1279.321\times10^{-3}T$
720-933.61 K: $\Delta Hf° = -4703.598 + 120.814\times10^{-3}T - 59.761\times10^{-6}T^{2} + 5098.800T^{-1}$
$\Delta Gf° = -4703.598 - 120.814\times10^{-3}T\ln T + 59.761\times10^{-6}T^{2} + 2549.400T^{-1} + 1599.459\times10^{-3}T$
933.61-1112 K: $\Delta Hf° = -4721.346 + 78.842\times10^{-3}T - 35.582\times10^{-6}T^{2} + 4855.200T^{-1}$
$\Delta Gf° = -4721.346 - 78.842\times10^{-3}T\ln T + 35.582\times10^{-6}T^{2} + 2427.600T^{-1} + 1354.133\times10^{-3}T$
1112-1310 K: $\Delta Hf° = -4724.322 - 6.442\times10^{-3}T + 23.722\times10^{-6}T^{2} + 4855.200T^{-1}$
$\Delta Gf° = -4724.322 + 6.442\times10^{-3}T\ln T - 23.722\times10^{-6}T^{2} + 2427.600T^{-1} + 824.581\times10^{-3}T$
1310-1700 K: $\Delta Hf° = -4645.142 - 91.070\times10^{-3}T + 44.674\times10^{-6}T^{2} - 745.800T^{-1}$
$\Delta Gf° = -4645.142 + 91.070\times10^{-3}T\ln T - 44.674\times10^{-6}T^{2} - 372.900T^{-1} + 185.776\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Koehler (276). Low-temperature heat capacities and entropy at 298 K from King (261). High-temperature data based on Bonnickson (53).

$CaB_2O_4(c,l)$
Calcium Borate
[Formation: $Ca(c,l) + 2B(\beta) + 2O_2(g) = CaB_2O_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.860	25.060	25.060	0	-485.580	-460.026	337.203
300	24.968	25.214	25.061	.046	-485.581	-459.864	335.006
400	29.598	33.126	26.108	2.807	-485.490	-451.304	246.578
500	32.459	40.055	28.221	5.917	-485.299	-442.775	193.535
600	34.638	46.173	30.713	9.276	-485.084	-434.293	158.189
700	36.423	51.651	33.320	12.832	-484.852	-425.848	132.954
720	36.726	52.681	33.843	13.563	-484.805	-424.160	128.748
720	36.726	52.681	33.843	13.563	-485.025	-424.160	128.748
800	37.936	56.616	35.926	16.552	-484.786	-417.407	114.029
900	39.233	61.161	38.481	20.412	-484.502	-408.986	99.314
1000	40.347	65.353	40.961	24.392	-484.300	-400.623	87.555
1100	41.293	69.244	43.357	28.476	-484.129	-392.272	77.936
1112	41.388	69.693	43.639	28.972	-484.113	-391.276	76.899
1112	41.388	69.693	43.639	28.972	-486.153	-391.276	76.899
1200	42.082	72.872	45.667	32.646	-485.679	-383.782	69.895
1300	42.720	76.267	47.892	36.887	-485.118	-375.308	63.094
1400	43.213	79.452	50.034	41.185	-484.544	-366.882	57.272
1435	43.351	80.520	50.764	42.700	-484.343	-363.943	55.428
1435	62.000	92.841	50.764	60.380	-466.663	-363.943	55.428
1500	62.000	95.588	52.648	64.410	-465.085	-359.323	52.353
1600	62.000	99.589	55.458	70.610	-462.695	-352.377	48.132
1700	62.000	103.348	58.166	76.810	-460.343	-345.542	44.422

Phase changes: 720 K, $\alpha - \beta$ transition point of Ca; $\Delta H^\circ = 0.220$ kcal/mol.
1112 K, melting point of Ca; $\Delta H^\circ = 2.040$ kcal/mol.
1435 K, melting point of CaB_2O_4; $\Delta H^\circ = 17.680$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1435 K: $C_p^\circ = 31.439 + 9.306\times10^{-3}T - 8.315\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 31.439\times10^{-3}T + 4.653\times10^{-6}T^2 + 8.315\times10^{2}T^{-1} - 12.576$
1435-1700 K: $C_p^\circ = 62.000$
$H^\circ - H^\circ_{298} = 62.000\times10^{-3}T - 28.590$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -487.861 + 3.702\times10^{-3}T - 0.307\times10^{-6}T^2 + 359.100T^{-1}$
$\Delta Gf^\circ = -487.861 - 3.702\times10^{-3}T\ln T + 0.307\times10^{-6}T^2 + 179.550T^{-1} + 112.341\times10^{-3}T$
720-1112 K: $\Delta Hf^\circ = -489.602 + 7.640\times10^{-3}T - 2.679\times10^{-6}T^2 + 298.100T^{-1}$
$\Delta Gf^\circ = -489.602 - 7.640\times10^{-3}T\ln T + 2.679\times10^{-6}T^2 + 149.050T^{-1} + 139.020\times10^{-3}T$
1112-1435 K: $\Delta Hf^\circ = -489.850 + 0.533\times10^{-3}T + 2.263\times10^{-6}T^2 + 298.100T^{-1}$
$\Delta Gf^\circ = -489.850 - 0.533\times10^{-3}T\ln T - 2.263\times10^{-6}T^2 + 149.050T^{-1} + 94.890\times10^{-3}T$
1435-1700 K: $\Delta Hf^\circ = -505.864 + 31.094\times10^{-3}T - 2.390\times10^{-6}T^2 - 533.400T^{-1}$
$\Delta Gf^\circ = -505.864 - 31.094\times10^{-3}T\ln T + 2.390\times10^{-6}T^2 - 266.700T^{-1} + 321.720\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Torgeson (501). Low-temperature heat capacities and entropy at 298 K from Kelley (251). High-temperature data based on King (269).

$CaB_4O_7(c,l)$
Calcium Diborate
[Formation: $Ca(c,l,g) + 4B(\beta) + 3.5O_2(g) = CaB_4O_7(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	37.750	32.200	32.200	0	-803.460	-757.277	555.092
300	37.960	32.430	32.200	.070	-803.466	-756.984	551.455
400	47.560	44.810	33.835	4.390	-803.516	-741.485	405.124
500	53.980	56.150	37.170	9.490	-803.245	-725.988	317.325
600	58.640	66.430	41.213	15.130	-802.832	-710.588	258.828
700	62.080	75.740	45.483	21.180	-802.309	-695.246	217.063
720	62.598	77.496	46.348	22.427	-802.198	-692.186	210.104
720	62.598	77.496	46.348	22.427	-802.418	-692.186	210.104
800	64.670	84.210	49.810	27.520	-801.911	-679.967	185.756
900	66.730	91.950	54.072	34.090	-801.276	-664.750	161.421
1000	68.550	99.070	58.210	40.860	-800.701	-649.616	141.972
1100	70.380	105.690	62.235	47.800	-800.141	-634.563	126.074
1112	70.636	106.455	62.709	48.646	-800.073	-632.762	124.361
1112	70.636	106.455	62.709	48.646	-802.113	-632.762	124.361
1200	72.510	111.900	66.108	54.950	-801.221	-619.375	112.802
1260	74.030	115.480	68.382	59.340	-800.560	-610.296	105.856
1260*	106.300	136.950	68.382	86.400	-773.500	-610.296	105.856
1300	106.300	140.270	70.539	90.650	-771.753	-605.137	101.732
1400	106.300	148.150	75.807	101.280	-767.439	-592.487	92.490
1500	106.300	155.490	80.883	111.910	-763.206	-580.137	84.525
1600	106.300	162.350	85.763	122.540	-759.057	-568.119	77.600
1700	106.300	168.790	90.455	133.170	-754.982	-556.288	71.515
1757	106.300	172.300	93.057	139.229	-752.694	-549.624	68.366
1757	106.300	172.300	93.057	139.229	-789.320	-549.624	68.366
1800	106.300	174.870	94.981	143.800	-787.524	-543.746	66.019

*On cooling, liquid solidifies to vitreous form.

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1260 K, melting point of CaB_4O_7; ΔH° = 27.060 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1260 K: $Cp° = 51.505 + 18.974\text{x}10^{-3}T - 17.256\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 51.505\text{x}10^{-3}T + 9.487\text{x}10^{-6}T^{2} + 17.256\text{x}10^{2}T^{-1} - 21.987$
1260-1800 K: $Cp° = 106.300$
$H°-H°_{298} = 106.300\text{x}10^{-3}T - 47.538$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -807.199 + 3.477\text{x}10^{-3}T + 2.388\text{x}10^{-6}T^{2} + 742.400T^{-1}$
$\Delta Gf° = -807.199 - 3.477\text{x}10^{-3}T\ln T - 2.388\text{x}10^{-6}T^{2} + 371.200T^{-1} + 183.785\text{x}10^{-3}T$
720-1112 K: $\Delta Hf° = -808.940 + 7.415\text{x}10^{-3}T + 0.017\text{x}10^{-6}T^{2} + 681.400T^{-1}$
$\Delta Gf° = -808.940 - 7.415\text{x}10^{-3}T\ln T - 0.017\text{x}10^{-6}T^{2} + 340.700T^{-1} + 210.463\text{x}10^{-3}T$
1112-1260 K: $\Delta Hf° = -809.188 + 0.308\text{x}10^{-3}T + 4.958\text{x}10^{-6}T^{2} + 681.400T^{-1}$
$\Delta Gf° = -809.188 - 0.308\text{x}10^{-3}T\ln T - 4.958\text{x}10^{-6}T^{2} + 340.700T^{-1} + 166.334\text{x}10^{-3}T$
1260-1757 K: $\Delta Hf° = -834.739 + 55.103\text{x}10^{-3}T - 4.529\text{x}10^{-6}T^{2} - 1044.200T^{-1}$
$\Delta Gf° = -834.739 - 55.103\text{x}10^{-3}T\ln T + 4.529\text{x}10^{-6}T^{2} - 522.100T^{-1} + 566.376\text{x}10^{-3}T$
1757-1800 K: $\Delta Hf° = -874.910 + 57.133\text{x}10^{-3}T - 4.536\text{x}10^{-6}T^{2} - 1044.200T^{-1}$
$\Delta Gf° = -874.910 - 57.133\text{x}10^{-3}T\ln T + 4.536\text{x}10^{-6}T^{2} - 522.100T^{-1} + 604.394\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Torgeson (501). Low-temperature heat capacities and entropy at 298 K from Kelley (251). High-temperature data based on King (269).

$Ca_2B_2O_5(c,l)$
Dicalcium Borate
[Formation: $2Ca(c,l,g) + 2B(\beta) + 2.5O_2(g) = Ca_2B_2O_5(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	35.200	34.680	34.680	0	-653.710	-620.755	455.020
300	35.320	34.900	34.680	.070	-653.705	-620.542	452.059
400	41.250	45.910	36.135	3.910	-653.506	-609.516	333.020
500	45.590	55.610	39.090	8.260	-653.083	-598.567	261.630
600	48.320	64.190	42.573	12.970	-652.579	-587.711	214.071
700	49.440	71.740	46.211	17.870	-652.124	-576.944	180.128
720	49.340	73.131	46.940	18.858	-652.053	-574.789	174.470
720	49.340	73.131	46.940	18.858	-652.493	-574.789	174.470
800	48.940	78.330	49.830	22.800	-652.213	-566.173	154.669
804	48.880	78.570	49.966	23.000	-652.200	-565.737	153.781
804	54.030	80.080	49.966	24.210	-650.990	-565.737	153.781
900	54.310	86.190	53.512	29.410	-650.396	-555.565	134.908
1000	54.600	91.920	57.060	34.860	-650.085	-545.070	119.123
1100	54.890	97.140	60.476	40.330	-649.974	-534.590	106.212
1112	54.925	97.736	60.875	40.989	-649.976	-533.342	104.820
1112	54.925	97.736	60.875	40.989	-654.056	-533.342	104.820
1200	55.180	101.930	63.738	45.830	-653.404	-523.816	95.399
1300	55.460	106.360	66.845	51.370	-652.673	-513.036	86.248
1400	55.750	110.480	69.816	56.930	-651.969	-502.319	78.415
1500	56.050	114.330	72.650	62.520	-651.279	-491.646	71.632
1585	56.290	117.430	74.976	67.290	-650.713	-482.656	66.551
1585	68.200	132.610	74.976	91.350	-626.653	-482.656	66.551
1600	68.200	133.250	75.519	92.370	-626.378	-481.294	65.741
1700	68.200	137.390	79.043	99.190	-624.547	-472.269	60.714
1757	68.200	139.631	80.964	103.077	-623.523	-467.145	58.106
1757	68.200	139.631	80.964	103.077	-696.775	-467.145	58.106
1800	68.200	141.280	82.386	106.010	-695.839	-461.470	56.029
1900	68.200	144.970	85.586	112.830	-693.692	-448.511	51.590

Phase changes:
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
804 K, α - β transition point of $Ca_2B_2O_5$; ΔH° = 1.210 kcal/mol.
2223 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1585 K, melting point of $Ca_2B_2O_5$; ΔH° = 24.060 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-804 K: $Cp° = 45.490 + 8.614\times10^{-3}T - 11.431\times10^{5}T^{-2}$
$H°- H°_{298} = 45.490\times10^{-3}T + 4.307\times10^{-6}T^2 + 11.431\times10^{2}T^{-1} - 17.780$
804-1585 K: $Cp° = 51.701 + 2.896\times10^{-3}T$
$H°- H°_{298} = 51.701\times10^{-3}T + 1.448\times10^{-6}T^2 - 18.294$
1585-1900 K: $Cp° = 68.200$
$H°- H°_{298} = 68.200\times10^{-3}T - 16.747$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -658.853 + 10.307\times10^{-3}T - 3.475\times10^{-6}T^2 + 709.100T^{-1}$
$\Delta Gf° = -658.853 - 10.307\times10^{-3}T\ln T + 3.475\times10^{-6}T^2 + 354.550T^{-1} + 181.481\times10^{-3}T$
720-804 K: $\Delta Hf° = -662.335 + 18.183\times10^{-3}T - 8.219\times10^{-6}T^2 + 587.100T^{-1}$
$\Delta Gf° = -662.335 - 18.183\times10^{-3}T\ln T + 8.219\times10^{-6}T^2 + 293.550T^{-1} + 234.838\times10^{-3}T$
804-1112 K: $\Delta Hf° = -662.848 + 24.394\times10^{-3}T - 11.078\times10^{-6}T^2 - 556.000T^{-1}$
$\Delta Gf° = -662.848 - 24.394\times10^{-3}T\ln T + 11.078\times10^{-6}T^2 - 278.000T^{-1} + 275.612\times10^{-3}T$
1112-1585 K: $\Delta Hf° = -663.344 + 10.180\times10^{-3}T - 1.194\times10^{-6}T^2 - 556.000T^{-1}$
$\Delta Gf° = -663.344 - 10.180\times10^{-3}T\ln T + 1.194\times10^{-6}T^2 - 278.000T^{-1} + 187.353\times10^{-3}T$
1585-1757 K: $\Delta Hf° = -661.798 + 26.679\times10^{-3}T - 2.641\times10^{-6}T^2 - 556.000T^{-1}$
$\Delta Gf° = -661.798 - 26.679\times10^{-3}T\ln T + 2.641\times10^{-6}T^2 - 278.000T^{-1} + 305.652\times10^{-3}T$
1757-1900 K: $\Delta Hf° = -742.140 + 30.739\times10^{-3}T - 2.655\times10^{-6}T^2 - 556.000T^{-1}$
$\Delta Gf° = -742.140 - 30.739\times10^{-3}T\ln T + 2.655\times10^{-6}T^2 - 278.000T^{-1} + 381.688\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Torgeson (501). Low-temperature heat capacities and entropy at 298 K from Kelley (251). High-temperature data based on King (269).

$Ca_3B_2O_6(c,l)$
Tricalcium Borate
[Formation: $3Ca(c,l,g) + 2B(\beta) + 3O_2(g) = Ca_3B_2O_6(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	44.900	43.890	43.890	0	-519.740	-479.262	351.304
300	45.100	44.170	43.903	.080	-519.742	-479.009	348.953
400	52.550	58.280	45.755	5.010	-519.424	-465.464	254.314
500	56.580	70.480	49.520	10.480	-518.890	-452.038	197.583
600	59.220	81.040	53.907	16.280	-518.357	-438.712	159.799
700	61.220	90.330	58.473	22.300	-517.903	-425.497	132.845
720	61.550	92.059	59.382	23.528	-517.826	-422.847	128.350
720	61.550	92.059	59.382	23.528	-518.486	-422.847	128.350
800	62.870	98.610	62.972	28.510	-518.077	-412.229	112.614
900	64.310	106.100	67.356	34.870	-517.727	-398.975	96.883
1000	65.630	112.950	71.580	41.370	-517.728	-385.838	84.324
1100	66.870	119.260	75.633	47.990	-517.914	-372.648	74.037
1112	67.012	119.986	76.107	48.793	-517.952	-371.079	72.930
1112	67.012	119.986	76.107	48.793	-524.072	-371.079	72.930
1200	68.050	125.130	79.513	54.740	-523.304	-358.995	65.381
1300	69.190	130.620	83.235	61.600	-522.380	-345.334	58.055
1400	70.310	135.790	86.804	68.580	-521.388	-331.745	51.787
1500	71.400	140.680	90.240	75.660	-520.344	-318.250	46.368
1600	72.480	145.320	93.533	82.860	-519.231	-304.836	41.638
1700	73.540	149.750	96.715	90.160	-518.061	-291.448	37.468
1757	74.148	152.183	98.474	94.368	-517.368	-283.838	35.306
1757	74.148	152.183	98.474	94.368	-627.246	-283.838	35.306
1760	74.180	152.310	98.565	94.590	-627.191	-283.249	35.172
1760	94.000	172.450	98.565	130.040	-591.741	-283.249	35.172
1800	94.000	174.560	100.227	133.800	-590.217	-276.151	33.529
1900	94.000	179.650	104.282	143.200	-586.436	-258.819	29.771

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.
1760 K, melting point of $Ca_3B_2O_6$; ΔH° = 35.450 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1760 K: $Cp^\circ = 56.926 + 10.048\times10^{-3}T - 13.437\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 56.926\times10^{-3}T + 5.024\times10^{-6}T^{2} + 13.437\times10^{2}T^{-1} - 21.926$
1760-1900 K: $Cp^\circ = 94.000$
$H^\circ - H^\circ_{298} = 94.000\times10^{-3}T - 35.400$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -526.687 + 14.297\times10^{-3}T - 5.579\times10^{-6}T^{2} + 948.100T^{-1}$
$\Delta Gf^\circ = -526.687 - 14.297\times10^{-3}T\ln T + 5.579\times10^{-6}T^{2} + 474.050T^{-1} + 233.527\times10^{-3}T$
720-1112 K: $\Delta Hf^\circ = -531.910 + 26.111\times10^{-3}T - 12.695\times10^{-6}T^{2} + 765.100T^{-1}$
$\Delta Gf^\circ = -531.910 - 26.111\times10^{-3}T\ln T + 12.695\times10^{-6}T^{2} + 382.550T^{-1} + 313.561\times10^{-3}T$
1112-1757 K: $\Delta Hf^\circ = -532.654 + 4.790\times10^{-3}T + 2.131\times10^{-6}T^{2} + 765.100T^{-1}$
$\Delta Gf^\circ = -532.654 - 4.790\times10^{-3}T\ln T - 2.131\times10^{-6}T^{2} + 382.550T^{-1} + 181.173\times10^{-3}T$
1757-1760 K: $\Delta Hf^\circ = -653.167 + 10.880\times10^{-3}T + 2.110\times10^{-6}T^{2} + 765.100T^{-1}$
$\Delta Gf^\circ = -653.167 - 10.880\times10^{-3}T\ln T - 2.110\times10^{-6}T^{2} + 382.550T^{-1} + 295.227\times10^{-3}T$
1760-1900 K: $\Delta Hf^\circ = -666.641 + 47.954\times10^{-3}T - 2.914\times10^{-6}T^{2} - 578.600T^{-1}$
$\Delta Gf^\circ = -666.641 - 47.954\times10^{-3}T\ln T + 2.914\times10^{-6}T^{2} - 289.300T^{-1} + 571.314\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Torgeson (501). Low-temperature heat capacities and entropy at 298 K from Kelley (251). High-temperature data based on King (269).

$CaC_2(c)$
Calcium Dicarbide
[Formation: $Ca(c,l) + 2C(c) = CaC_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.990	16.720	16.720	0	-14.300	-15.503	11.364
300	15.020	16.813	16.720	.028	-14.291	-15.510	11.299
400	16.273	21.324	17.326	1.599	-13.824	-15.987	8.735
500	17.043	25.044	18.510	3.267	-13.433	-16.578	7.246
600	17.522	28.197	19.867	4.998	-13.140	-17.231	6.276
700	17.767	30.920	21.257	6.764	-12.954	-17.937	5.600
720	17.790	31.420	21.531	7.120	-12.930	-18.075	5.486
720	17.033	33.253	21.531	8.440	-11.830	-18.075	5.486
800	17.157	35.055	22.796	9.807	-11.795	-18.769	5.127
900	17.313	37.084	24.272	11.531	-11.855	-19.624	4.765
1000	17.469	38.917	25.647	13.270	-12.078	-20.495	4.479
1100	17.625	40.589	26.931	15.024	-12.399	-21.299	4.232
1112	17.644	40.780	27.079	15.236	-12.445	-21.401	4.206
1112	17.644	40.780	27.079	15.236	-14.485	-21.401	4.206
1200	17.781	42.129	28.133	16.795	-14.490	-21.970	4.001
1300	17.937	43.559	29.266	18.581	-14.504	-22.594	3.798

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
720 K, α - β transition point of CaC_2; ΔH° = 1.320 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-720 K: $Cp° = 16.647 + 2.378\times10^{-3}T - 2.101\times10^{5}T^{-2}$
$H°- H°_{298} = 16.647\times10^{-3}T + 1.189\times10^{-6}T^{2} + 2.101\times10^{2}T^{-1} - 5.774$
720-1300 K: $Cp° = 15.881 + 1.580\times10^{-3}T + 0.077\times10^{5}T^{-2}$
$H°- H°_{298} = 15.881\times10^{-3}T + 0.790\times10^{-6}T^{2} - 0.077\times10^{2}T^{-1} - 3.393$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -15.518 + 5.780\times10^{-3}T - 2.913\times10^{-6}T^{2} - 73.500T^{-1}$
$\Delta Gf° = -15.518 - 5.780\times10^{-3}T\ln T + 2.913\times10^{-6}T^{2} - 36.750T^{-1} + 32.526\times10^{-3}T$
720-1112 K: $\Delta Hf° = -14.878 + 8.952\times10^{-3}T - 5.684\times10^{-6}T^{2} - 352.300T^{-1}$
$\Delta Gf° = -14.878 - 8.952\times10^{-3}T\ln T + 5.684\times10^{-6}T^{2} - 176.150T^{-1} + 50.780\times10^{-3}T$
1112-1300 K: $\Delta Hf° = -15.126 + 1.845\times10^{-3}T - 0.742\times10^{-6}T^{2} - 352.300T^{-1}$
$\Delta Gf° = -15.126 - 1.845\times10^{-3}T\ln T + 0.742\times10^{-6}T^{2} - 176.150T^{-1} + 6.651\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Kelley (241). High-temperature data based on Moore (338).

$CaCO_3$(calcite)
Calcium Carbonate, Calcite
[Formation: $Ca(c,l) + C(c) + 1.5O_2(g) = CaCO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	19.950	21.920	21.920	0	-288.610	-269.857	197.808
300	20.010	22.040	21.920	.037	-288.607	-269.738	196.501
400	23.180	28.290	22.750	2.216	-288.353	-263.482	143.958
500	24.990	33.670	24.408	4.631	-287.995	-257.306	112.467
600	26.260	38.340	26.347	7.196	-287.623	-251.198	91.498
700	27.280	42.470	28.364	9.874	-287.268	-245.163	76.543
720	27.458	43.241	28.767	10.421	-287.201	-243.958	74.050
720	27.458	43.241	28.767	10.421	-287.421	-243.958	74.050
800	28.170	46.170	30.360	12.648	-287.116	-239.141	65.330
900	28.990	49.540	32.310	15.507	-286.776	-233.154	56.617
1000	29.750	52.630	34.186	18.444	-286.534	-227.224	49.659
1100	30.480	55.500	35.995	21.456	-286.331	-221.290	43.966
1112	30.566	55.831	36.207	21.822	-286.311	-220.586	43.353
1112	30.566	55.831	36.207	21.822	-288.351	-220.586	43.353
1200	31.200	58.190	37.741	24.539	-287.844	-215.262	39.204

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 23.837 + 6.428\times10^{-3}T - 5.160\times10^{5}T^{-2}$
$H° - H°_{298} = 23.837\times10^{-3}T + 3.214\times10^{-6}T^{2} + 5.160\times10^{2}T^{-1} - 9.123$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -291.345 + 5.643\times10^{-3}T - 0.877\times10^{-6}T^{2} + 336.900T^{-1}$
$\Delta Gf° = -291.345 - 5.643\times10^{-3}T\ln T + 0.877\times10^{-6}T^{2} + 168.450T^{-1} + 102.066\times10^{-3}T$
720-1112 K: $\Delta Hf° = -293.086 + 9.581\times10^{-3}T - 3.248\times10^{-6}T^{2} + 275.900T^{-1}$
$\Delta Gf° = -293.086 - 9.581\times10^{-3}T\ln T + 3.248\times10^{-6}T^{2} + 137.950T^{-1} + 128.745\times10^{-3}T$
1112-1200 K: $\Delta Hf° = -293.334 + 2.474\times10^{-3}T + 1.694\times10^{-6}T^{2} + 275.900T^{-1}$
$\Delta Gf° = -293.334 - 2.474\times10^{-3}T\ln T - 1.694\times10^{-6}T^{2} + 137.950T^{-1} + 84.615\times10^{-3}T$

Source: Data from Chang (74).

$CaCO_3$(aragonite)
Calcium Carbonate, Aragonite
[Formation: $Ca(c) + C(c) + 1.5O_2(g) = CaCO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	19.670	21.030	21.030	0	-288.660	-269.641	197.650
300	20.130	21.150	21.030	.037	-288.658	-269.521	196.343
400	22.150	27.190	21.843	2.139	-288.480	-263.169	143.787
500	23.860	32.320	23.432	4.444	-288.232	-256.868	112.275
600	25.280	36.800	25.297	6.902	-287.967	-250.618	91.286
700	26.570	40.790	27.226	9.495	-287.698	-244.417	76.309

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 19.596 + 10.776\times10^{-3}T - 2.809\times10^{5}T^{-2}$

$H°-H°_{298} = 19.596\times10^{-3}T + 5.388\times10^{-6}T^{2} + 2.809\times10^{2}T^{-1} - 7.264$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -289.535 + 1.402\times10^{-3}T + 1.297\times10^{-6}T^{2} + 101.800T^{-1}$

$\Delta Gf° = -289.535 - 1.402\times10^{-3}T\ln T - 1.297\times10^{-6}T^{2} + 50.900T^{-1} + 74.526\times10^{-3}T$

Source: Data from Chang (74).

$CaFe_2O_4$(c,l)
Calcium Ferrite
[Formation: Ca(c,l,g) + 2Fe(c) + $2O_2$(g) = $CaFe_2O_4$(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^\circ_{298})/T$	$H°-H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	36.720	34.740	34.740	0	-363.370	-337.655	247.504
300	36.780	34.970	34.740	.070	-363.359	-337.492	245.860
400	39.110	45.920	36.220	3.880	-362.837	-328.950	179.728
500	40.360	54.790	39.070	7.860	-362.326	-320.537	140.105
600	41.230	62.230	42.330	11.940	-361.914	-312.218	113.724
700	41.930	68.640	45.640	16.100	-361.632	-303.963	94.900
720	42.054	69.823	46.295	16.940	-361.596	-302.313	91.763
720	42.054	69.823	46.295	16.940	-361.816	-302.313	91.763
800	42.550	74.280	48.880	20.320	-361.704	-295.714	80.784
900	43.130	79.330	51.986	24.610	-361.776	-287.445	69.800
1000	43.710	83.900	54.950	28.950	-362.310	-279.180	61.014
1043	43.955	85.745	56.182	30.835	-362.841	-275.596	57.747
1100	44.280	88.090	57.772	33.350	-363.279	-270.806	53.804
1112	44.350	88.571	58.102	33.882	-363.345	-269.803	53.026
1112	44.350	88.571	58.102	33.882	-365.385	-269.803	53.026
1185	44.773	91.406	60.066	37.138	-365.381	-263.528	48.602
1185	44.773	91.406	60.066	37.138	-365.811	-263.528	48.602
1200	44.860	91.970	60.462	37.810	-365.743	-262.236	47.759
1300	45.450	95.580	63.026	42.320	-365.285	-253.628	42.638
1400	46.060	98.980	65.480	46.900	-364.815	-245.065	38.256
1500	46.680	102.170	67.817	51.530	-364.347	-236.526	34.461
1510	46.750	102.480	68.042	52.000	-364.296	-235.669	34.109
1510	54.900	119.610	68.042	77.870	-338.426	-235.669	34.109
1600	54.900	122.800	71.044	82.810	-337.283	-229.597	31.361
1667	54.900	125.044	73.161	86.488	-336.458	-225.082	29.509
1667	54.900	125.044	73.161	86.488	-336.858	-225.082	29.509
1700	54.900	126.120	74.179	88.300	-336.511	-222.873	28.652
1757	54.900	127.933	75.895	91.429	-335.925	-219.074	27.250
1757	54.900	127.933	75.895	91.429	-372.551	-219.074	27.250
1800	54.900	129.260	77.154	93.790	-372.037	-215.291	26.140

Phase changes:
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1510 K, incongruent melting point of $CaFe_2O_4$; ΔH° = 25.870 kcal/mol. Selected temperature is midrange. Liquidus temperature could be as high as 1600 K.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1510 K: $Cp° = 39.337 + 4.838\times10^{-3}T - 3.608\times10^{5}T^{-2}$
$H°-H^\circ_{298} = 39.337\times10^{-3}T + 2.419\times10^{-6}T^{2} + 3.608\times10^{2}T^{-1} - 13.153$
1510-1800 K: $Cp° = 54.900$
$H°-H^\circ_{298} = 54.900\times10^{-3}T - 5.029$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -371.239 + 21.488\times10^{-3}T - 13.299\times10^{-6}T^{2} + 788.400T^{-1}$
$\Delta Gf° = -371.239 - 21.488\times10^{-3}T\ln T + 13.299\times10^{-6}T^{2} + 394.200T^{-1} + 226.672\times10^{-3}T$
720-1043 K: $\Delta Hf° = -372.980 + 25.426\times10^{-3}T - 15.671\times10^{-6}T^{2} + 727.400T^{-1}$
$\Delta Gf° = -372.980 - 25.426\times10^{-3}T\ln T + 15.671\times10^{-6}T^{2} + 363.700T^{-1} + 253.350\times10^{-3}T$
1043-1112 K: $\Delta Hf° = -325.858 - 62.536\times10^{-3}T + 25.751\times10^{-6}T^{2} + 270.400T^{-1}$
$\Delta Gf° = -325.858 + 62.536\times10^{-3}T\ln T - 25.751\times10^{-6}T^{2} + 135.200T^{-1} - 359.739\times10^{-3}T$
1112-1185 K: $\Delta Hf° = -326.106 - 69.643\times10^{-3}T + 30.693\times10^{-6}T^{2} + 270.400T^{-1}$
$\Delta Gf° = -326.106 + 69.643\times10^{-3}T\ln T - 30.693\times10^{-6}T^{2} + 135.200T^{-1} - 403.868\times10^{-3}T$
1185-1510 K: $\Delta Hf° = -373.334 + 6.867\times10^{-3}T - 0.689\times10^{-6}T^{2} + 508.400T^{-1}$
$\Delta Gf° = -373.334 - 6.867\times10^{-3}T\ln T + 0.689\times10^{-6}T^{2} + 254.200T^{-1} + 140.214\times10^{-3}T$
1510-1667 K: $\Delta Hf° = -365.210 + 22.430\times10^{-3}T - 3.108\times10^{-6}T^{2} + 147.600T^{-1}$
$\Delta Gf° = -365.210 - 22.430\times10^{-3}T\ln T + 3.108\times10^{-6}T^{2} + 73.800T^{-1} + 245.179\times10^{-3}T$
1667-1757 K: $\Delta Hf° = -530.999 + 119.424\times10^{-3}T - 22.370\times10^{-6}T^{2} + 95546.000T^{-1}$
$\Delta Gf° = -530.999 - 119.424\times10^{-3}T\ln T + 22.370\times10^{-6}T^{2} + 47773.000T^{-1} + 1014.935\times10^{-3}T$
1757-1800 K: $\Delta Hf° = -571.170 + 121.454\times10^{-3}T - 22.377\times10^{-6}T^{2} + 95546.000T^{-1}$
$\Delta Gf° = -571.170 - 121.454\times10^{-3}T\ln T + 22.377\times10^{-6}T^{2} + 47773.000T^{-1} + 1052.953\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Koehler (276). Low-temperature heat capacities and entropy at 298 K from King (258). High-temperature data based on Bonnickson (51).

$Ca_2Fe_2O_5$(c,l)
Dicalcium Ferrite
[Formation: $2Ca(c,l,g) + 2Fe(c,l) + 2.5O_2(g) = Ca_2Fe_2O_5(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	46.100	45.110	45.110	0	-512.040	-479.147	351.220
300	46.250	45.400	45.133	.080	-512.036	-478.948	348.909
400	51.960	59.660	47.010	5.060	-511.315	-468.006	255.703
500	54.460	71.560	50.780	10.390	-510.463	-457.289	199.878
600	55.880	81.620	55.087	15.920	-509.662	-446.714	162.713
700	56.780	90.310	59.524	21.550	-509.031	-436.293	136.215
720	56.902	91.911	60.402	22.687	-508.932	-434.209	131.799
720	56.902	91.911	60.402	22.687	-509.372	-434.209	131.799
800	57.390	97.930	63.855	27.260	-508.978	-425.876	116.342
900	57.840	104.720	68.031	33.020	-508.797	-415.477	100.890
1000	58.180	110.830	72.010	38.820	-509.233	-405.128	88.540
1043	58.292	113.282	73.661	41.324	-509.754	-400.642	83.949
1100	58.440	116.390	75.790	44.660	-510.208	-394.652	78.409
1112	58.465	117.024	76.232	45.361	-510.286	-393.402	77.317
1112	58.465	117.024	76.232	45.361	-514.366	-393.402	77.317
1185	58.618	120.742	78.860	49.630	-514.169	-385.468	71.091
1185	58.618	120.742	78.860	49.630	-514.599	-385.468	71.091
1200	58.650	121.480	79.388	50.510	-514.492	-383.836	69.905
1300	58.820	126.180	82.811	56.380	-513.802	-372.978	62.702
1400	58.950	130.550	86.071	62.270	-513.154	-362.175	56.537
1500	59.050	134.620	89.173	68.170	-512.552	-351.421	51.201
1600	59.140	138.430	92.130	74.080	-511.996	-340.694	46.536
1667	59.180	140.860	94.041	78.047	-511.647	-333.512	43.724
1667	59.180	140.860	94.041	78.047	-512.047	-333.512	43.724
1700	59.200	142.020	94.961	80	-511.935	-329.979	42.421
1750	59.220	143.730	96.326	82.960	-511.776	-324.621	40.540
1750	74.700	164.230	96.326	118.830	-475.906	-324.621	40.540
1757	74.700	164.528	96.598	119.353	-475.777	-324.018	40.303
1757	74.700	164.528	96.598	119.353	-549.029	-324.018	40.303
1800	74.700	166.340	98.251	122.560	-548.075	-318.472	38.667
1811	74.700	166.795	98.666	123.382	-547.838	-317.076	38.264
1811	74.700	166.795	98.666	123.382	-554.438	-317.076	38.264
1900	74.700	170.380	101.943	130.030	-552.626	-305.458	35.135

Phase changes:
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1750 K, melting point of $Ca_2Fe_2O_5$; ΔH° = 35.870 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1750 K: $Cp^\circ = 58.969 + 0.374\times10^{-3}T - 11.539\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 58.969\times10^{-3}T + 0.187\times10^{-6}T^2 + 11.539\times10^{2}T^{-1} - 21.468$
1750-1900 K: $Cp^\circ = 74.700$
$H^\circ - H^\circ_{298} = 74.700\times10^{-3}T - 11.895$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -525.882 + 33.674\times10^{-3}T - 18.353\times10^{-6}T^2 + 1619.900T^{-1}$
$\Delta Gf^\circ = -525.882 - 33.674\times10^{-3}T\ln T + 18.353\times10^{-6}T^2 + 809.950T^{-1} + 334.025\times10^{-3}T$
720-1043 K: $\Delta Hf^\circ = -529.364 + 41.550\times10^{-3}T - 23.097\times10^{-6}T^2 + 1497.900T^{-1}$
$\Delta Gf^\circ = -529.364 - 41.550\times10^{-3}T\ln T + 23.097\times10^{-6}T^2 + 748.950T^{-1} + 387.382\times10^{-3}T$
1043-1112 K: $\Delta Hf^\circ = -482.242 - 46.412\times10^{-3}T + 18.326\times10^{-6}T^2 + 1040.900T^{-1}$
$\Delta Gf^\circ = -482.242 + 46.412\times10^{-3}T\ln T - 18.326\times10^{-6}T^2 + 520.450T^{-1} - 225.707\times10^{-3}T$
1112-1185 K: $\Delta Hf^\circ = -482.738 - 60.626\times10^{-3}T + 28.209\times10^{-6}T^2 + 1040.900T^{-1}$
$\Delta Gf^\circ = -482.738 + 60.626\times10^{-3}T\ln T - 28.209\times10^{-6}T^2 + 520.450T^{-1} - 313.966\times10^{-3}T$
1185-1667 K: $\Delta Hf^\circ = -529.966 + 15.884\times10^{-3}T - 3.173\times10^{-6}T^2 + 1278.900T^{-1}$
$\Delta Gf^\circ = -529.966 - 15.884\times10^{-3}T\ln T + 3.173\times10^{-6}T^2 + 639.450T^{-1} + 230.115\times10^{-3}T$
1667-1750 K: $\Delta Hf^\circ = -695.756 + 112.878\times10^{-3}T - 22.434\times10^{-6}T^2 + 96677.300T^{-1}$
$\Delta Gf^\circ = -695.756 - 112.878\times10^{-3}T\ln T + 22.434\times10^{-6}T^2 + 48338.650T^{-1} + 999.872\times10^{-3}T$
1750-1757 K: $\Delta Hf^\circ = -686.183 + 128.609\times10^{-3}T - 22.622\times10^{-6}T^2 + 95523.400T^{-1}$
$\Delta Gf^\circ = -686.183 - 128.609\times10^{-3}T\ln T + 22.622\times10^{-6}T^2 + 47761.700T^{-1} + 1111.732\times10^{-3}T$
1757-1811 K: $\Delta Hf^\circ = -766.525 + 132.669\times10^{-3}T - 22.635\times10^{-6}T^2 + 95523.400T^{-1}$
$\Delta Gf^\circ = -766.525 - 132.669\times10^{-3}T\ln T + 22.635\times10^{-6}T^2 + 47761.700T^{-1} + 1187.768\times10^{-3}T$
1811-1900 K: $\Delta Hf^\circ = -594.825 + 24.685\times10^{-3}T - 1.271\times10^{-6}T^2 - 113.000T^{-1}$
$\Delta Gf^\circ = -594.825 - 24.685\times10^{-3}T\ln T + 1.271\times10^{-6}T^2 - 56.500T^{-1} + 336.172\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Koehler (276). Low-temperature heat capacities and entropy at 298 K from King (258). High-temperature data based on Bonnickson (51).

$(Ca_{0.9516}, Mg_{0.583})Fe^{2+}_{0.7134}Fe^{3+}_{0.0934}Mn_{0.1366}(Si_2O_6)(c)$

Hedenbergite

[Formation: $0.9516Ca(c,l) + 0.0583Mg(c,l) + 0.8068Fe(c) + 2Si(c) + 3O_2(g) + 0.1366Mn(c) = hedenbergite(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	41.491	41.218	41.218	0	-680.960	-641.897	470.517
300	41.690	41.475	41.218	.077	-680.962	-641.653	467.438
400	47.619	54.315	42.930	4.554	-680.844	-628.564	343.427
500	52.046	65.447	46.343	9.552	-680.426	-615.534	269.046
600	54.814	75.205	50.358	14.908	-679.865	-602.607	219.497
700	56.284	83.778	54.534	20.471	-679.303	-589.782	184.136
720	56.427	85.366	55.368	21.598	-679.202	-587.222	178.244
720	56.427	85.366	55.368	21.598	-679.411	-587.222	178.244
800	56.999	91.346	58.672	26.139	-679.010	-576.999	157.627
900	57.423	98.085	62.683	31.862	-678.676	-564.253	137.018
922	57.506	99.473	63.544	33.126	-678.639	-561.457	133.085
922	57.506	99.473	63.544	33.126	-678.764	-561.457	133.085
980	57.725	102.988	65.776	36.468	-678.741	-554.080	123.564
980	57.725	102.988	65.776	36.468	-678.814	-554.080	123.564
1000	57.801	104.155	66.532	37.623	-678.834	-551.535	120.536
1043	57.952	106.592	68.134	40.112	-678.962	-546.059	114.420
1100	58.152	109.681	70.207	43.421	-679.049	-538.804	107.049
1112	58.179	110.312	70.637	44.119	-679.060	-537.279	105.594
1112	58.179	110.312	70.637	44.119	-681.001	-537.279	105.594
1185	58.342	114.017	73.195	48.374	-680.763	-527.852	97.351
1185	58.342	114.017	73.195	48.374	-680.936	-527.852	97.351
1200	58.375	114.751	73.710	49.249	-680.863	-525.916	95.781

Phase changes:
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 55.023 + 4.522\times10^{-3}T - 13.227\times10^{5}T^{-2}$
$H° - H°_{298} = 55.023\times10^{-3}T + 2.261\times10^{-6}T^{2} + 13.227\times10^{2}T^{-1} - 21.042$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -689.601 + 17.438\times10^{-3}T - 7.608\times10^{-6}T^{2} + 1227.828T^{-1}$
$\Delta Gf° = -689.601 - 17.438\times10^{-3}T\ln T + 7.608\times10^{-6}T^{2} + 613.914T^{-1} + 250.177\times10^{-3}T$
720-922 K: $\Delta Hf° = -691.258 + 21.185\times10^{-3}T - 9.865\times10^{-6}T^{2} + 1169.781T^{-1}$
$\Delta Gf° = -691.258 - 21.185\times10^{-3}T\ln T + 9.865\times10^{-6}T^{2} + 584.890T^{-1} + 275.564\times10^{-3}T$
922-980 K: $\Delta Hf° = -691.335 + 21.135\times10^{-3}T - 9.847\times10^{-6}T^{2} + 1154.523T^{-1}$
$\Delta Gf° = -691.335 - 21.135\times10^{-3}T\ln T + 9.847\times10^{-6}T^{2} + 577.262T^{-1} + 275.329\times10^{-3}T$
980-1043 K: $\Delta Hf° = -691.278 + 20.837\times10^{-3}T - 9.691\times10^{-6}T^{2} + 1166.380T^{-1}$
$\Delta Gf° = -691.278 - 20.837\times10^{-3}T\ln T + 9.691\times10^{-6}T^{2} + 583.190T^{-1} + 273.365\times10^{-3}T$
1043-1112 K: $\Delta Hf° = -672.269 - 14.647\times10^{-3}T + 7.019\times10^{-6}T^{2} + 982.026T^{-1}$
$\Delta Gf° = -672.269 + 14.647\times10^{-3}T\ln T - 7.019\times10^{-6}T^{2} + 491.013T^{-1} + 26.045\times10^{-3}T$
1112-1185 K: $\Delta Hf° = -672.505 - 21.410\times10^{-3}T + 11.722\times10^{-6}T^{2} + 982.026T^{-1}$
$\Delta Gf° = -672.505 + 21.410\times10^{-3}T\ln T - 11.722\times10^{-6}T^{2} + 491.013T^{-1} - 15.948\times10^{-3}T$
1185-1200 K: $\Delta Hf° = -691.556 + 9.454\times10^{-3}T - 0.938\times10^{-6}T^{2} + 1078.036T^{-1}$
$\Delta Gf° = -691.556 - 9.454\times10^{-3}T\ln T + 0.938\times10^{-6}T^{2} + 539.018T^{-1} + 203.534\times10^{-3}T$

Source: Data from Bennington (28).

$CaH(g)$
Calcium Hydride (ideal gas)
[Formation: $Ca(c,l,g) + 0.5H_2(g) = CaH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.145	48.215	48.215	0	54.830	48.070	-35.236
300	7.150	48.260	48.217	.013	54.826	48.029	-34.989
400	7.440	50.355	48.500	.742	54.592	45.799	-25.023
500	7.745	52.048	49.044	1.502	54.359	43.627	-19.069
600	8.009	53.484	49.667	2.290	54.113	41.505	-15.118
700	8.225	54.736	50.305	3.102	53.842	39.419	-12.307
720	8.260	54.968	50.431	3.267	53.782	39.012	-11.842
720	8.260	54.968	50.431	3.267	53.562	39.012	-11.842
800	8.398	55.846	50.930	3.933	53.354	37.408	-10.219
900	8.539	56.843	51.532	4.780	53.035	35.449	-8.608
1000	8.656	57.749	52.109	5.640	52.589	33.500	-7.321
1100	8.755	58.579	52.660	6.511	52.070	31.617	-6.282
1112	8.765	58.674	52.724	6.616	52.001	31.389	-6.169
1112	8.765	58.674	52.724	6.616	49.961	31.389	-6.169
1200	8.842	59.344	53.185	7.391	49.796	29.927	-5.450
1300	8.920	60.055	53.687	8.279	49.611	28.278	-4.754
1400	8.992	60.719	54.165	9.175	49.429	26.645	-4.159
1500	9.059	61.342	54.624	10.077	49.247	25.018	-3.645
1600	9.124	61.928	55.062	10.986	49.068	23.407	-3.197
1700	9.186	62.483	55.482	11.902	48.890	21.819	-2.805
1757	9.220	62.787	55.714	12.427	48.789	20.911	-2.601
1757	9.220	62.787	55.714	12.427	12.163	20.911	-2.601
1800	9.245	63.010	55.886	12.824	12.173	21.158	-2.569
1900	9.302	63.512	56.275	13.751	12.198	21.656	-2.491
2000	9.355	63.990	56.648	14.684	12.224	22.153	-2.421

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.637 + 0.974\times10^{-3}T - 0.696\times10^{5}T^{-2}$
$H°- H°_{298} = 7.637\times10^{-3}T + 0.487\times10^{-6}T^2 + 0.696\times10^{2}T^{-1} - 2.554$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = 54.396 + 0.578\times10^{-3}T - 2.293\times10^{-6}T^2 + 138.850T^{-1}$
$\Delta Gf° = 54.396 - 0.578\times10^{-3}T\ln T + 2.293\times10^{-6}T^2 + 69.425T^{-1} - 19.386\times10^{-3}T$
720-1112 K: $\Delta Hf° = 52.655 + 4.516\times10^{-3}T - 4.665\times10^{-6}T^2 + 77.850T^{-1}$
$\Delta Gf° = 52.655 - 4.516\times10^{-3}T\ln T + 4.665\times10^{-6}T^2 + 38.925T^{-1} + 7.292\times10^{-3}T$
1112-1757 K: $\Delta Hf° = 52.407 - 2.591\times10^{-3}T + 0.278\times10^{-6}T^2 + 77.850T^{-1}$
$\Delta Gf° = 52.407 + 2.591\times10^{-3}T\ln T - 0.278\times10^{-6}T^2 + 38.925T^{-1} - 36.838\times10^{-3}T$
1757-2000 K: $\Delta Hf° = 12.236 - 0.561\times10^{-3}T + 0.271\times10^{-6}T^2 + 77.850T^{-1}$
$\Delta Gf° = 12.236 + 0.561\times10^{-3}T\ln T - 0.271\times10^{-6}T^2 + 38.925T^{-1} + 1.180\times10^{-3}T$

Source: Data from Gurvich (196).

$CaH_2(c,l)$
Calcium Dihydride
[Formation: $Ca(c,l,g) + H_2(g) = CaH_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	9.799	9.895	9.895	0	-42.300	-32.982	24.176
300	9.816	9.956	9.896	.018	-42.306	-32.924	23.985
400	10.703	12.901	10.291	1.044	-42.590	-29.752	16.255
500	11.590	15.385	11.067	2.159	-42.817	-26.516	11.590
600	12.478	17.576	11.973	3.362	-42.998	-23.236	8.464
700	13.365	19.566	12.917	4.654	-43.140	-19.936	6.224
720	13.543	19.945	13.107	4.923	-43.166	-19.270	5.849
720	13.543	19.945	13.107	4.923	-43.386	-19.270	5.849
800	14.253	21.409	13.865	6.035	-43.431	-16.585	4.531
900	15.140	23.139	14.800	7.505	-43.482	-13.210	3.208
1000	16.028	24.780	15.717	9.063	-43.590	-9.860	2.155
1053	16.498	25.620	16.194	9.925	-43.644	-8.069	1.675
1053	16.500	27.139	16.194	11.525	-42.044	-8.069	1.675
1100	16.500	27.860	16.678	12.300	-42.106	-6.552	1.302
1112	16.500	28.039	16.800	12.498	-42.126	-6.169	1.212
1112	16.500	28.039	16.800	12.498	-44.166	-6.169	1.212
1200	16.500	29.295	17.670	13.950	-43.978	-3.168	.577
1273	16.500	30.270	18.365	15.155	-43.828	-.691	.119
1273	17.925	34.400	18.365	20.413	-38.570	-.691	.119
1300	17.925	34.776	18.701	20.897	-38.477	.112	-.019
1400	17.925	36.104	19.898	22.689	-38.141	3.069	-.479
1500	17.925	37.341	21.020	24.482	-37.815	5.997	-.874
1600	17.925	38.498	22.077	26.274	-37.500	8.903	-1.216
1700	17.925	39.585	23.075	28.067	-37.194	11.805	-1.518
1757	17.925	40.177	23.620	29.089	-37.024	13.442	-1.672
1757	17.925	40.177	23.620	29.089	-73.650	13.442	-1.672
1800	17.925	40.610	24.021	29.860	-73.438	15.604	-1.895
1900	17.925	41.579	24.920	31.652	-72.951	20.539	-2.362
2000	17.925	42.498	25.776	33.445	-72.473	25.447	-2.781

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1053 K, α - β transition point of CaH_2; ΔH° = 1.600 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1273 K, melting point of CaH_2; ΔH° = 5.258 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1053 K: $Cp^\circ = 7.152 + 8.876\times10^{-3}T$
$H^\circ - H^\circ_{298} = 7.152\times10^{-3}T + 4.438\times10^{-6}T^2 - 2.527$
1053-1273 K: $Cp^\circ = 16.500$
$H^\circ - H^\circ_{298} = 16.500\times10^{-3}T - 5.850$
1273-2000 K: $Cp^\circ = 17.925$
$H^\circ - H^\circ_{298} = 17.925\times10^{-3}T - 2.406$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -41.754 - 3.135\times10^{-3}T + 1.449\times10^{-6}T^2 + 77.500T^{-1}$
$\Delta Gf^\circ = -41.754 + 3.135\times10^{-3}T\ln T - 1.449\times10^{-6}T^2 + 38.750T^{-1} + 11.555\times10^{-3}T$
720-1053 K: $\Delta Hf^\circ = -43.495 + 0.803\times10^{-3}T - 0.923\times10^{-6}T^2 + 16.500T^{-1}$
$\Delta Gf^\circ = -43.495 - 0.803\times10^{-3}T\ln T + 0.923\times10^{-6}T^2 + 8.250T^{-1} + 38.233\times10^{-3}T$
1053-1112 K: $\Delta Hf^\circ = -46.818 + 10.151\times10^{-3}T - 5.361\times10^{-6}T^2 + 16.500T^{-1}$
$\Delta Gf^\circ = -46.818 - 10.151\times10^{-3}T\ln T + 5.361\times10^{-6}T^2 + 8.250T^{-1} + 101.772\times10^{-3}T$
1112-1273 K: $\Delta Hf^\circ = -47.066 + 3.044\times10^{-3}T - 0.419\times10^{-6}T^2 + 16.500T^{-1}$
$\Delta Gf^\circ = -47.066 - 3.044\times10^{-3}T\ln T + 0.419\times10^{-6}T^2 + 8.250T^{-1} + 57.642\times10^{-3}T$
1273-1757 K: $\Delta Hf^\circ = -43.622 + 4.469\times10^{-3}T - 0.419\times10^{-6}T^2 + 16.500T^{-1}$
$\Delta Gf^\circ = -43.622 - 4.469\times10^{-3}T\ln T + 0.419\times10^{-6}T^2 + 8.250T^{-1} + 65.124\times10^{-3}T$
1757-2000 K: $\Delta Hf^\circ = -83.793 + 6.499\times10^{-3}T - 0.426\times10^{-6}T^2 + 16.500T^{-1}$
$\Delta Gf^\circ = -83.793 - 6.499\times10^{-3}T\ln T + 0.426\times10^{-6}T^2 + 8.250T^{-1} + 103.142\times10^{-3}T$

Source: Data from Gurvich (196).

$CaMoO_4(c)$
Calcium Molybdate
[Formation: $Ca(c,l) + Mo(c) + 2O_2(g) = CaMoO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	27.330	29.300	29.300	0	-368.400	-342.908	251.355
300	27.403	29.469	29.300	.051	-368.397	-342.749	249.689
400	30.611	37.821	30.418	2.961	-368.110	-334.237	182.616
500	32.926	44.913	32.625	6.144	-367.639	-325.820	142.414
600	34.717	51.080	35.198	9.529	-367.073	-317.507	115.650
700	36.142	56.543	37.864	13.075	-366.452	-309.298	96.566
720	36.370	57.564	38.398	13.800	-366.326	-307.664	93.388
720	36.370	57.564	38.398	13.800	-366.546	-307.664	93.388
800	37.281	61.446	40.511	16.748	-365.990	-301.151	82.270
900	38.178	65.891	43.088	20.523	-365.312	-293.071	71.166
1000	38.858	69.951	45.574	24.377	-364.730	-285.095	62.307
1100	39.339	73.679	47.963	28.288	-364.208	-277.155	55.065
1112	39.374	74.106	48.242	28.760	-364.151	-276.211	54.286
1112	39.374	74.106	48.242	28.760	-366.191	-276.211	54.286
1200	39.632	77.115	50.250	32.238	-365.438	-269.118	49.012
1300	39.745	80.293	52.441	36.208	-364.595	-261.127	43.899

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 30.882 + 8.514\text{x}10^{-3}T - 5.414\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 30.882\text{x}10^{-3}T + 4.257\text{x}10^{-6}T^{2} + 5.414\text{x}10^{2}T^{-1} - 11.402$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -372.720 + 8.214\text{x}10^{-3}T - 0.504\text{x}10^{-6}T^{2} + 571.200T^{-1}$
$\Delta Gf^\circ = -372.720 - 8.214\text{x}10^{-3}T\ln T + 0.504\text{x}10^{-6}T^{2} + 285.600T^{-1} + 143.426\text{x}10^{-3}T$
720-1112 K: $\Delta Hf^\circ = -374.461 + 12.152\text{x}10^{-3}T - 2.876\text{x}10^{-6}T^{2} + 510.200T^{-1}$
$\Delta Gf^\circ = -374.461 - 12.152\text{x}10^{-3}T\ln T + 2.876\text{x}10^{-6}T^{2} + 255.100T^{-1} + 170.104\text{x}10^{-3}T$
1112-1300 K: $\Delta Hf^\circ = -374.709 + 5.045\text{x}10^{-3}T + 2.066\text{x}10^{-6}T^{2} + 510.200T^{-1}$
$\Delta Gf^\circ = -374.709 - 5.045\text{x}10^{-3}T\ln T - 2.066\text{x}10^{-6}T^{2} + 255.100T^{-1} + 125.975\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Weller (522). High-temperature data based on Zhidikova (546).

$Ca_3N_2(c)$
Tricalcium Dinitride
[Formation: $3Ca(c) + N_2(g) = Ca_3N_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	26.500	25.000	25.000	0	-103.000	-87.917	64.444
300	26.600	25.160	25.000	.050	-102.996	-87.818	63.975
400	29.400	33.220	26.070	2.860	-102.731	-82.792	45.235
500	31.500	40.020	28.200	5.910	-102.313	-77.860	34.032
600	33.400	45.940	30.673	9.160	-101.828	-73.007	26.592
700	35.200	51.230	33.244	12.590	-101.321	-68.263	21.312
720	35.540	52.226	33.758	13.297	-101.223	-67.308	20.431
720	35.540	52.226	33.758	13.297	-101.883	-67.308	20.431
800	36.900	56.040	35.790	16.200	-101.352	-63.482	17.342
900	38.600	60.480	38.291	19.970	-100.771	-58.739	14.264

Phase change: 720 K, α – β transition point of Ca; ΔH° = 0.220 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp° = 24.725 + 15.726x10^{-3}T - 2.580x10^{5}T^{-2}$
$H°- H°_{298} = 24.725x10^{-3}T + 7.863x10^{-6}T^{2} + 2.580x10^{2}T^{-1} - 8.936$

Formation equations (kcal/mol):

298.15-720 K: $ΔHf° = -106.469 + 6.715x10^{-3}T - 0.436x10^{-6}T^{2} + 448.900T^{-1}$
$ΔGf° = -106.469 - 6.715x10^{-3}TlnT + 0.436x10^{-6}T^{2} + 224.450T^{-1} + 97.829x10^{-3}T$
720-900 K: $ΔHf° = -111.692 + 18.529x10^{-3}T - 7.552x10^{-6}T^{2} + 265.900T^{-1}$
$ΔGf° = -111.692 - 18.529x10^{-3}TlnT + 7.552x10^{-6}T^{2} + 132.950T^{-1} + 177.864x10^{-3}T$

Sources: Enthalpy of formation from Parker (391). Entropy at 298 K from Rossini (431). Other data based on the three average heat capacity measurements of Sato (434).

$Ca(NO_3)_2(c)$
Calcium Nitrate
[Formation: $Ca(c,l) + N_2(g) + 3O_2(g) = Ca(NO_3)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	35.700	46.170	46.170	0	-224.280	-177.603	130.185
300	35.820	46.391	46.171	.066	-224.277	-177.312	129.170
400	41.486	57.528	47.651	3.951	-223.835	-161.711	88.354
500	46.071	67.288	50.622	8.333	-222.992	-146.271	63.934
600	50.280	76.064	54.142	13.153	-221.834	-131.029	47.727
700	54.312	84.119	57.858	18.383	-220.397	-116.010	36.219
720	55.099	85.660	58.609	19.477	-220.078	-113.028	34.308
720	55.099	85.660	58.609	19.477	-220.298	-113.028	34.308
800	58.249	91.629	61.614	24.012	-218.871	-101.184	27.642

Phase change: 720 K, $\alpha - \beta$ transition point of Ca; $\Delta H° = 0.220$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 29.308 + 36.890\text{x}10^{-3}T - 4.096\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 29.308\text{x}10^{-3}T + 18.445\text{x}10^{-6}T^{2} + 4.096\text{x}10^{2}T^{-1} - 11.752$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -225.841 - 2.730\text{x}10^{-3}T + 13.777\text{x}10^{-6}T^{2} + 342.900T^{-1}$

$\Delta Gf° = -225.841 + 2.730\text{x}10^{-3}T\ln T - 13.777\text{x}10^{-6}T^{2} + 171.450T^{-1} + 148.415\text{x}10^{-3}T$

720-800 K: $\Delta Hf° = -227.582 + 1.208\text{x}10^{-3}T + 11.405\text{x}10^{-6}T^{2} + 281.900T^{-1}$

$\Delta Gf° = -227.582 - 1.208\text{x}10^{-3}T\ln T - 11.405\text{x}10^{-6}T^{2} + 140.950T^{-1} + 175.093\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Shomate (454). High-temperature data based on Shomate (450).

$CaOH(g)$
Calcium Monohydroxide (ideal gas)
[Formation: $Ca(c,l,g) + 0.5O_2(g) + 0.5H_2(g) = CaOH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	10.665	56.252	56.252	0	-46.340	-48.190	35.324
300	10.686	56.318	56.252	.020	-46.344	-48.201	35.114
400	11.505	59.516	56.683	1.133	-46.549	-48.788	26.656
500	11.965	62.137	57.519	2.309	-46.731	-49.328	21.561
600	12.254	64.346	58.478	3.521	-46.931	-49.826	18.149
700	12.463	66.251	59.455	4.757	-47.167	-50.296	15.703
720	12.498	66.603	59.649	5.007	-47.220	-50.381	15.293
720	12.498	66.603	59.649	5.007	-47.440	-50.381	15.293
800	12.638	67.927	60.412	6.012	-47.629	-50.696	13.849
900	12.797	69.425	61.332	7.284	-47.930	-51.047	12.396
1000	12.947	70.781	62.209	8.572	-48.363	-51.389	11.231
1100	13.090	72.022	63.047	9.873	-48.871	-51.666	10.265
1112	13.106	72.164	63.144	10.030	-48.938	-51.702	10.161
1112	13.106	72.164	63.144	10.030	-50.978	-51.702	10.161
1200	13.225	73.167	63.843	11.189	-51.133	-51.753	9.425
1300	13.353	74.231	64.602	12.518	-51.305	-51.798	8.708
1400	13.471	75.225	65.325	13.860	-51.473	-51.828	8.091
1500	13.581	76.158	66.017	15.212	-51.639	-51.852	7.555
1600	13.682	77.037	66.678	16.575	-51.804	-51.863	7.084
1700	13.774	77.870	67.312	17.948	-51.965	-51.853	6.666
1757	13.822	78.324	67.661	18.735	-52.056	-51.847	6.449
1757	13.822	78.324	67.661	18.735	-88.682	-51.847	6.449
1800	13.859	78.659	67.920	19.330	-88.666	-50.913	6.182
1900	13.936	79.411	68.506	20.720	-88.625	-48.818	5.615
2000	14.008	80.128	69.069	22.117	-88.585	-46.725	5.106

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.020 + 1.072\times10^{-3}T - 1.489\times10^{5}T^{-2}$
$H°-H°_{298} = 12.020\times10^{-3}T + 0.536\times10^{-6}T^{2} + 1.489\times10^{2}T^{-1} - 4.131$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -47.175 + 1.346\times10^{-3}T - 2.495\times10^{-6}T^{2} + 195.550T^{-1}$
$\Delta Gf° = -47.175 - 1.346\times10^{-3}T\ln T + 2.495\times10^{-6}T^{2} + 97.775T^{-1} + 2.421\times10^{-3}T$
720-1112 K: $\Delta Hf° = -48.916 + 5.284\times10^{-3}T - 4.867\times10^{-6}T^{2} + 134.550T^{-1}$
$\Delta Gf° = -48.916 - 5.284\times10^{-3}T\ln T + 4.867\times10^{-6}T^{2} + 67.275T^{-1} + 29.099\times10^{-3}T$
1112-1757 K: $\Delta Hf° = -49.164 - 1.823\times10^{-3}T + 0.075\times10^{-6}T^{2} + 134.550T^{-1}$
$\Delta Gf° = -49.164 + 1.823\times10^{-3}T\ln T - 0.075\times10^{-6}T^{2} + 67.275T^{-1} - 15.030\times10^{-3}T$
1757-2000 K: $\Delta Hf° = -89.336 + 0.207\times10^{-3}T + 0.068\times10^{-6}T^{2} + 134.550T^{-1}$
$\Delta Gf° = -89.336 - 0.207\times10^{-3}T\ln T - 0.068\times10^{-6}T^{2} + 67.275T^{-1} + 22.988\times10^{-3}T$

Source: Data from Chase (82) who estimated all except enthalpy of formation at 298 K.

$Ca(OH)_2(c)$
Calcium Dihydroxide

[Formation: $Ca(c,l) + H_2(g) + O_2(g) = Ca(OH)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	20.910	19.930	19.930	0	-235.680	-214.743	157.409
300	20.980	20.060	19.930	.039	-235.678	-214.612	156.343
400	23.520	26.487	20.789	2.279	-235.458	-207.618	113.436
500	24.840	31.891	22.485	4.703	-235.107	-200.699	87.724
600	25.680	36.495	24.445	7.230	-234.719	-193.851	70.609
700	26.460	40.513	26.460	9.837	-234.324	-187.076	58.407
720	26.594	41.260	26.861	10.368	-234.246	-185.724	56.374
720	26.594	41.260	26.861	10.368	-234.466	-185.724	56.374
800	27.130	44.092	28.444	12.518	-234.113	-180.325	49.262

Phase change: 720 K, α – β transition point of Ca; ΔH° = 0.220 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K:
$$Cp° = 24.667 + 3.828\times10^{-3}T - 4.355\times10^{5}T^{-2}$$
$$H°-H°_{298} = 24.667\times10^{-3}T + 1.914\times10^{-6}T^{2} + 4.355\times10^{2}T^{-1} - 8.985$$

Formation equations (kcal/mol):

298.15-720 K:
$$\Delta Hf° = -239.241 + 7.150\times10^{-3}T - 1.578\times10^{-6}T^{2} + 467.800T^{-1}$$
$$\Delta Gf° = -239.241 - 7.150\times10^{-3}T\ln T + 1.578\times10^{-6}T^{2} + 233.900T^{-1} + 119.800\times10^{-3}T$$

720-800 K:
$$\Delta Hf° = -240.982 + 11.088\times10^{-3}T - 3.950\times10^{-6}T^{2} + 406.800T^{-1}$$
$$\Delta Gf° = -240.982 - 11.088\times10^{-3}T\ln T + 3.950\times10^{-6}T^{2} + 203.400T^{-1} + 146.478\times10^{-3}T$$

Source: Data from Chase (82).

$Ca(OH)_2(g)$
Calcium Dihydroxide (ideal gas)
[Formation: $Ca(c,l,g) + H_2(g) + O_2(g) = Ca(OH)_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	17.555	68.234	68.234	0	-145.980	-139.445	102.215
300	17.595	68.343	68.234	.033	-145.984	-139.403	101.554
400	19.199	73.649	68.947	1.881	-146.156	-137.181	74.951
500	20.079	78.037	70.339	3.849	-146.261	-134.926	58.975
600	20.627	81.749	71.939	5.886	-146.363	-132.647	48.316
700	21.026	84.960	73.576	7.969	-146.492	-130.357	40.699
720	21.093	85.553	73.900	8.390	-146.524	-129.892	39.427
720	21.093	85.553	73.900	8.390	-146.744	-129.892	39.427
800	21.360	87.790	75.179	10.089	-146.842	-128.012	34.971
900	21.667	90.324	76.724	12.240	-147.026	-125.634	30.508
1000	21.959	92.622	78.200	14.422	-147.337	-123.259	26.938
1100	22.238	94.728	79.608	16.632	-147.719	-120.831	24.007
1112	22.270	94.969	79.772	16.899	-147.771	-120.542	23.691
1112	22.270	94.969	79.772	16.899	-149.811	-120.542	23.691
1200	22.504	96.674	80.950	18.869	-149.852	-118.224	21.531
1300	22.755	98.485	82.230	21.132	-149.891	-115.587	19.432
1400	22.988	100.180	83.452	23.419	-149.924	-112.946	17.631
1500	23.205	101.774	84.621	25.729	-149.951	-110.309	16.072
1600	23.404	103.278	85.741	28.059	-149.975	-107.669	14.707
1700	23.586	104.702	86.814	30.409	-149.994	-105.012	13.500
1757	23.681	105.482	87.407	31.756	-150.004	-103.505	12.875
1757	23.681	105.482	87.407	31.756	-186.630	-103.505	12.875
1800	23.752	106.055	87.846	32.776	-186.552	-101.439	12.316
1900	23.904	107.344	88.839	35.159	-186.368	-96.717	11.125
2000	24.042	108.573	89.795	37.556	-186.185	-92.003	10.053

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 720 K, α − β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 20.183 + 2.070\times10^{-3}T - 2.885\times10^{5}T^{-2}$
$H°-H°_{298} = 20.183\times10^{-3}T + 1.035\times10^{-6}T^{2} + 2.885\times10^{2}T^{-1} - 7.077$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -147.632 + 2.666\times10^{-3}T - 2.457\times10^{-6}T^{2} + 320.800T^{-1}$
$\Delta Gf° = -147.632 - 2.666\times10^{-3}T\ln T + 2.457\times10^{-6}T^{2} + 160.400T^{-1} + 40.113\times10^{-3}T$
720-1112 K: $\Delta Hf° = -149.373 + 6.604\times10^{-3}T - 4.829\times10^{-6}T^{2} + 259.800T^{-1}$
$\Delta Gf° = -149.373 - 6.604\times10^{-3}T\ln T + 4.829\times10^{-6}T^{2} + 129.900T^{-1} + 66.791\times10^{-3}T$
1112-1757 K: $\Delta Hf° = -149.621 - 0.503\times10^{-3}T + 0.113\times10^{-6}T^{2} + 259.800T^{-1}$
$\Delta Gf° = -149.621 + 0.503\times10^{-3}T\ln T - 0.113\times10^{-6}T^{2} + 129.900T^{-1} + 22.662\times10^{-3}T$
1757-2000 K: $\Delta Hf° = -189.793 + 1.527\times10^{-3}T + 0.106\times10^{-6}T^{2} + 259.800T^{-1}$
$\Delta Gf° = -189.793 - 1.527\times10^{-3}T\ln T - 0.106\times10^{-6}T^{2} + 129.900T^{-1} + 60.680\times10^{-3}T$

Source: Data from Chase (82) who estimated all except enthalpy of formation at 298 K.

$Ca_2P_2O_7(c,l)$
Calcium Pyrophosphate
[Formation: $2Ca(c,l) + 2P(c,l,1/4P_4(g)) + 3.5O_2(g) = Ca_2P_2O_7(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	44.880	45.230	45.230	0	-798.000	-748.564	548.706
300	45.050	45.510	45.243	.080	-798.009	-748.260	545.100
317.3	46.263	48.070	45.328	.870	-798.054	-745.388	513.402
317.3	46.263	48.070	45.328	.870	-798.368	-745.388	513.402
400	52.060	59.600	47.100	5.000	-798.359	-731.568	399.705
500	55.930	71.660	50.840	10.410	-798.051	-714.904	312.480
550	57.325	77.071	52.983	13.249	-797.825	-706.625	280.783
550	57.325	77.071	52.983	13.249	-803.641	-706.625	280.783
600	58.720	82.120	55.203	16.150	-803.233	-697.822	254.178
700	61.000	91.340	59.711	22.140	-802.375	-680.324	212.404
720	61.402	93.064	60.614	23.364	-802.202	-676.832	205.444
720	61.402	93.064	60.614	23.364	-802.642	-676.832	205.444
800	63.010	99.620	64.195	28.340	-801.855	-662.897	181.093
900	64.860	107.150	68.561	34.730	-800.898	-645.558	156.761
1000	66.620	114.080	72.770	41.310	-800.079	-628.378	137.330
1100	68.300	120.510	76.828	48.050	-799.304	-611.249	121.442
1112	68.498	121.252	77.304	48.871	-799.214	-609.208	119.731
1112	68.498	121.252	77.304	48.871	-803.294	-609.208	119.731
1200	69.950	126.520	80.712	54.970	-801.902	-593.891	108.161
1300	71.560	132.180	84.457	62.040	-800.208	-576.629	96.939
1400	73.150	137.550	88.064	69.280	-798.374	-559.503	87.341
1413.15	73.360	138.220	88.518	70.240	-798.126	-557.247	86.180
1413.15	76.850	139.350	88.518	71.830	-796.536	-557.247	86.180
1500	76.850	143.930	91.597	78.500	-794.583	-542.613	79.058
1600	76.850	148.890	95.028	86.180	-792.356	-525.898	71.833
1626.15	76.850	150.140	95.901	88.200	-791.765	-521.544	70.093
1626.15	96.850	164.880	95.901	112.170	-767.795	-521.544	70.093
1700	96.850	169.180	98.992	119.320	-764.689	-510.408	65.617

Phase changes:
317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P; ΔH° = 2.908 kcal/mol of P.
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1413.15 K, α - β transition point of $Ca_2P_2O_7$; ΔH° = 1.590 kcal/mol.
1626.15 K, melting point of $Ca_2P_2O_7$; ΔH° = 23.970 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1413.15 K: $Cp^\circ = 52.607 + 15.056\times10^{-3}T - 10.506\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 52.607\times10^{-3}T + 7.528\times10^{-6}T^2 + 10.506\times10^{2}T^{-1} - 19.878$
1413.15-1626.15 K: $Cp^\circ = 76.852$
$H^\circ - H^\circ_{298} = 76.852\times10^{-3}T - 36.773$
1626.15-1700 K: $Cp^\circ = 96.850$
$H^\circ - H^\circ_{298} = 96.850\times10^{-3}T - 45.323$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf^\circ = -804.482 + 12.042\times10^{-3}T - 5.742\times10^{-6}T^2 + 1014.400T^{-1}$
$\Delta Gf^\circ = -804.482 - 12.042\times10^{-3}T\ln T + 5.742\times10^{-6}T^2 + 507.200T^{-1} + 248.741\times10^{-3}T$
317.3-550 K: $\Delta Hf^\circ = -803.855 + 7.056\times10^{-3}T + 0.627\times10^{-6}T^2 + 1014.400T^{-1}$
$\Delta Gf^\circ = -803.855 - 7.056\times10^{-3}T\ln T - 0.627\times10^{-6}T^2 + 507.200T^{-1} + 220.069\times10^{-3}T$
550- 720 K: $\Delta Hf^\circ = -810.776 + 9.732\times10^{-3}T + 0.619\times10^{-6}T^2 + 813.800T^{-1}$
$\Delta Gf^\circ = -810.776 - 9.732\times10^{-3}T\ln T - 0.619\times10^{-6}T^2 + 406.900T^{-1} + 249.864\times10^{-3}T$
720-1112 K: $\Delta Hf^\circ = -814.258 + 17.608\times10^{-3}T - 4.124\times10^{-6}T^2 + 691.800T^{-1}$
$\Delta Gf^\circ = -814.258 - 17.608\times10^{-3}T\ln T + 4.124\times10^{-6}T^2 + 345.900T^{-1} + 303.220\times10^{-3}T$
1112-1413.15 K: $\Delta Hf^\circ = -814.754 + 3.394\times10^{-3}T + 5.760\times10^{-6}T^2 + 691.800T^{-1}$
$\Delta Gf^\circ = -814.754 - 3.394\times10^{-3}T\ln T - 5.760\times10^{-6}T^2 + 345.900T^{-1} + 214.962\times10^{-3}T$
1413.15-1626.15 K: $\Delta Hf^\circ = -831.649 + 27.639\times10^{-3}T - 1.769\times10^{-6}T^2 - 358.800T^{-1}$
$\Delta Gf^\circ = -831.649 - 27.639\times10^{-3}T\ln T + 1.769\times10^{-6}T^2 - 179.400T^{-1} + 392.405\times10^{-3}T$
1626.15-1700 K: $\Delta Hf^\circ = -840.199 + 47.637\times10^{-3}T - 1.769\times10^{-6}T^2 - 358.800T^{-1}$
$\Delta Gf^\circ = -840.199 - 47.637\times10^{-3}T\ln T + 1.769\times10^{-6}T^2 - 179.400T^{-1} + 545.527\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Parker (391). Other data based on Egan (134).

$Ca_3(PO_4)_2(\beta)$
β-Calcium Phosphate

[Formation: $3Ca(c,l) + 2P(c,l,1/4P_4(g)) + 4O_2(g) = Ca_3(PO_4)_2(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	54.450	56.400	56.400	0	-984.900	-928.526	680.619
300	54.590	56.740	56.407	.100	-984.907	-928.175	676.167
317.3	55.687	59.831	56.510	1.054	-984.953	-924.900	637.044
317.3	55.687	59.831	56.510	1.054	-985.267	-924.900	637.044
400	60.930	73.360	58.610	5.900	-985.347	-909.142	496.726
500	65.990	87.510	63.010	12.250	-985.108	-890.116	389.064
550	68.270	93.911	65.530	15.609	-984.885	-880.649	349.933
550	68.270	93.911	65.530	15.609	-990.701	-880.649	349.933
600	70.550	99.950	68.150	19.080	-990.262	-870.662	317.134
700	74.880	111.160	73.517	26.350	-989.244	-850.829	265.637
720	75.720	113.281	74.592	27.856	-989.022	-846.866	257.056
720	75.720	113.281	74.592	27.856	-989.682	-846.866	257.056
800	79.080	121.430	78.868	34.050	-988.590	-831.048	227.029
900	83.210	130.980	84.136	42.160	-987.130	-811.396	197.031
1000	87.290	139.960	89.270	50.690	-985.722	-791.996	173.088
1100	91.350	148.470	94.270	59.620	-984.203	-772.691	153.517
1112	91.834	149.464	94.860	60.719	-984.016	-770.400	151.411
1112	91.834	149.464	94.860	60.719	-990.136	-770.400	151.411
1200	95.380	156.590	99.123	68.960	-987.591	-753.104	137.157
1300	99.410	164.390	103.852	78.700	-984.355	-733.702	123.345
1373	102.330	169.900	107.220	86.060	-981.765	-719.697	114.558
1373	80	172.770	107.220	90	-977.825	-719.697	114.558
1400	80	174.330	108.501	92.160	-977.433	-714.628	111.557
1500	80	179.840	113.067	100.160	-975.997	-695.908	101.392
1600	80	185.010	117.410	108.160	-974.589	-677.299	92.514

Phase changes:
317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P; ΔH° = 2.908 kcal/mol of P.
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1373 K, α - β transition point of $Ca_3(PO_4)_2$; ΔH° = 3.940 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1373 K: $Cp° = 48.069 + 39.710\times10^{-3}T - 4.839\times10^{5}T^{-2}$
$H°-H°_{298} = 48.069\times10^{-3}T + 19.855\times10^{-6}T^{2} + 4.839\times10^{2}T^{-1} - 17.720$
1373-1600: $Cp° = 80.000$
$H°-H°_{298} = 80.000$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -986.882 + 0.058\times10^{-3}T + 3.763\times10^{-6}T^{2} + 486.100T^{-1}$
$\Delta Gf° = -986.882 - 0.058\times10^{-3}T\ln T - 3.763\times10^{-6}T^{2} + 243.050T^{-1} + 194.447\times10^{-3}T$
317.3-550 K: $\Delta Hf° = -986.255 - 4.928\times10^{-3}T + 10.133\times10^{-6}T^{2} + 486.100T^{-1}$
$\Delta Gf° = -986.255 + 4.928\times10^{-3}T\ln T - 10.133\times10^{-6}T^{2} + 243.050T^{-1} + 165.774\times10^{-3}T$
550-720 K: $\Delta Hf° = -993.176 - 2.252\times10^{-3}T + 10.125\times10^{-6}T^{2} + 285.500T^{-1}$
$\Delta Gf° = -993.176 + 2.252\times10^{-3}T\ln T - 10.125\times10^{-6}T^{2} + 142.750T^{-1} + 195.569\times10^{-3}T$
720-1112 K: $\Delta Hf° = -998.399 + 9.562\times10^{-3}T + 3.009\times10^{-6}T^{2} + 102.500T^{-1}$
$\Delta Gf° = -998.399 - 9.562\times10^{-3}T\ln T - 3.009\times10^{-6}T^{2} + 51.250T^{-1} + 275.604\times10^{-3}T$
1112-1373 K: $\Delta Hf° = -999.143 - 11.759\times10^{-3}T + 17.835\times10^{-6}T^{2} + 102.500T^{-1}$
$\Delta Gf° = -999.143 + 11.759\times10^{-3}T\ln T - 17.835\times10^{-6}T^{2} + 51.250T^{-1} + 143.216\times10^{-3}T$
1373-1600 K: $\Delta Hf° = -1001.263 + 20.172\times10^{-3}T - 2.020\times10^{-6}T^{2} - 381.400T^{-1}$
$\Delta Gf° = -1001.263 - 20.172\times10^{-3}T\ln T + 2.020\times10^{-6}T^{2} - 190.700T^{-1} + 348.321\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Southard (469). High-temperature data based on Kelley (243) and Britzke (58).

$Ca_{10}(PO_4)_6F_2(c)$
Fluorapatite

[Formation: $10Ca(c,l) + 6P(c,l,1/4P_4(g)) + F_2(g) + 12O_2(g) = Ca_{10}(PO_4)_6F_2(fluorapatite)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	179.500	185.500	185.500	0	-3285.000	-3103.330	2274.773
300	180.240	186.610	185.510	.330	-3285.016	-3102.197	2259.920
317.3	184.854	196.845	185.852	3.488	-3285.094	-3091.646	2129.436
317.3	184.854	196.845	185.852	3.488	-3286.036	-3091.646	2129.436
400	206.910	242.550	192.950	19.840	-3285.611	-3041.004	1661.506
500	220.970	290.370	207.770	41.300	-3283.931	-2980.038	1302.557
550	225.420	311.682	216.250	52.488	-3282.903	-2949.758	1172.111
550	225.420	311.682	216.250	52.488	-3300.351	-2949.758	1172.111
600	229.870	331.490	225.040	63.870	-3298.827	-2917.949	1062.848
700	236.340	367.440	242.883	87.190	-3295.843	-2854.766	891.287
720	237.376	374.113	246.436	91.927	-3295.285	-2842.133	862.694
720	237.376	374.113	246.436	91.927	-3297.485	-2842.133	862.694
800	241.520	399.340	260.478	111.090	-3294.909	-2791.664	762.637
900	245.930	428.050	277.528	135.470	-3292.160	-2728.770	662.627
1000	249.880	454.170	293.910	160.260	-3290.564	-2666.451	582.745
1100	253.530	478.160	309.578	185.440	-3289.530	-2604.063	517.373
1112	253.943	480.913	311.412	188.485	-3289.459	-2596.639	510.331
1112	253.943	480.913	311.412	188.485	-3309.859	-2596.639	510.331
1200	256.970	500.370	324.570	210.960	-3305.871	-2540.363	462.657
1300	260.250	521.070	338.893	236.830	-3301.108	-2476.762	416.376
1400	263.440	540.470	352.606	263.010	-3296.142	-2413.523	376.763
1500	266.540	558.750	365.743	289.510	-3290.937	-2350.708	342.494
1600	269.590	576.050	378.350	316.320	-3285.509	-2288.222	312.553

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P; ΔH° = 2.908 kcal/mol of P.
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 227.152 + 27.746x10^{-3}T - 50.139x10^{5}T^{-2}$
$H°-H°_{298} = 227.152x10^{-3}T + 13.873x10^{-6}T^{2} + 50.139x10^{2}T^{-1} - 85.775$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -3319.507 + 70.780x10^{-3}T - 37.147x10^{-6}T^{2} + 4981.000T^{-1}$
$\Delta Gf° = -3319.507 - 70.780x10^{-3}TlnT + 37.147x10^{-6}T^{2} + 2490.500T^{-1} + 1089.245x10^{-3}T$
317.3-550 K: $\Delta Hf° = -3317.627 + 55.822x10^{-3}T - 18.037x10^{-6}T^{2} + 4981.000T^{-1}$
$\Delta Gf° = -3317.627 - 55.822x10^{-3}TlnT + 18.037x10^{-6}T^{2} + 2490.500T^{-1} + 1003.228x10^{-3}T$
550-720 K: $\Delta Hf° = -3338.389 + 63.850x10^{-3}T - 18.061x10^{-6}T^{2} + 4379.200T^{-1}$
$\Delta Gf° = -3338.389 - 63.850x10^{-3}TlnT + 18.061x10^{-6}T^{2} + 2189.600T^{-1} + 1092.614x10^{-3}T$
720-1112 K: $\Delta Hf° = -3355.799 + 103.230x10^{-3}T - 41.781x10^{-6}T^{2} + 3769.200T^{-1}$
$\Delta Gf° = -3355.799 - 103.230x10^{-3}TlnT + 41.781x10^{-6}T^{2} + 1884.600T^{-1} + 1359.396x10^{-3}T$
1112-1600 K: $\Delta Hf° = -3358.280 + 32.160x10^{-3}T + 7.639x10^{-6}T^{2} + 3769.200T^{-1}$
$\Delta Gf° = -3358.280 - 32.160x10^{-3}TlnT - 7.639x10^{-6}T^{2} + 1884.600T^{-1} + 918.103x10^{-3}T$

Sources: Enthalpy of formation from Parker (391). Other data based on Egan (136).

$Ca_{10}(PO_4)_6(OH)_2(c)$
Hydroxyapatite

[Formation: $10Ca(c,l) + 6P(c,l,1/4P_4(g)) + H_2(g) + 13O_2(g) = Ca_{10}(PO_4)_6(OH)_2$(hydroxyapatite)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	184.100	186.600	186.600	0	-3221.000	-3030.186	2221.158
300	184.700	187.740	186.740	.300	-3221.058	-3029.035	2206.622
317.3	189.475	198.229	187.083	3.537	-3221.169	-3017.953	2078.678
317.3	189.475	198.229	187.083	3.537	-3222.111	-3017.953	2078.678
400	212.300	244.960	194.210	20.300	-3221.798	-2964.701	1619.816
500	228.700	294.270	209.470	42.400	-3220.104	-2900.644	1267.854
550	233.500	316.364	218.173	54.005	-3218.970	-2868.805	1139.943
550	233.500	316.364	218.173	54.005	-3236.418	-2868.805	1139.943
600	238.300	336.890	227.223	65.800	-3234.795	-2835.452	1032.800
700	244.800	374.130	245.559	90.000	-3231.563	-2769.165	864.561
720	245.960	381.043	249.226	94.908	-3230.962	-2755.924	836.526
720	245.960	381.043	249.226	94.908	-3233.162	-2755.924	836.526
800	250.600	407.190	263.815	114.700	-3230.471	-2703.102	738.444
900	256.700	437.050	281.383	140.100	-3227.356	-2637.169	640.384
1000	263.300	464.440	298.340	166.100	-3225.215	-2571.897	562.080
1100	269.900	489.840	314.567	192.800	-3223.340	-2506.586	498.006
1112	270.620	492.772	316.475	196.043	-3223.153	-2498.822	491.106
1112	270.620	492.772	316.475	196.043	-3243.553	-2498.822	491.106
1200	275.900	513.590	330.173	220.100	-3238.594	-2440.079	444.393
1300	281.000	535.880	345.188	247.900	-3232.608	-2373.837	399.073
1400	286.100	556.880	359.523	276.300	-3226.142	-2307.942	360.281
1500	293.000	576.840	373.373	305.200	-3219.271	-2242.681	326.754

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P; ΔH° = 2.908 kcal/mol of P.
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 221.065 + 47.896\times10^{-3}T - 45.554\times10^{5}T^{-2}$
$H°-H°_{298} = 221.065\times10^{-3}T + 23.948\times10^{-6}T^2 + 45.554\times10^{2}T^{-1} - 83.318$

Formation equations (kcal/mol):

298.15-317.3 K: $ΔHf° = -3251.681 + 59.515\times10^{-3}T - 27.820\times10^{-6}T^2 + 4594.300T^{-1}$
$ΔGf° = -3251.681 - 59.515\times10^{-3}T\ln T + 27.820\times10^{-6}T^2 + 2297.150T^{-1} + 1047.853\times10^{-3}T$
317.3-550 K: $ΔHf° = -3249.801 + 44.557\times10^{-3}T - 8.710\times10^{-6}T^2 + 4594.300T^{-1}$
$ΔGf° = -3249.801 - 44.557\times10^{-3}T\ln T + 8.710\times10^{-6}T^2 + 2297.150T^{-1} + 961.834\times10^{-3}T$
550-720 K: $ΔHf° = -3270.562 + 52.585\times10^{-3}T - 8.734\times10^{-6}T^2 + 3992.500T^{-1}$
$ΔGf° = -3270.562 - 52.585\times10^{-3}T\ln T + 8.734\times10^{-6}T^2 + 1996.250T^{-1} + 1051.221\times10^{-3}T$
720-1112 K: $ΔHf° = -3287.972 + 91.965\times10^{-3}T - 32.454\times10^{-6}T^2 + 3382.500T^{-1}$
$ΔGf° = -3287.972 - 91.965\times10^{-3}T\ln T + 32.454\times10^{-6}T^2 + 1691.250T^{-1} + 1318.001\times10^{-3}T$
1112-1500 K: $ΔHf° = -3290.452 + 20.895\times10^{-3}T + 16.966\times10^{-6}T^2 + 3382.500T^{-1}$
$ΔGf° = -3290.452 - 20.895\times10^{-3}T\ln T - 16.966\times10^{-6}T^2 + 1691.250T^{-1} + 876.707\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Egan (136). High-temperature data based on Egan (135).

$CaSO_3(c)$
Calcium Sulfite
[Reaction: $Ca(c,l) + 0.5S_2(g) + 1.5O_2(g) = CaSO_3(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	21.920	24.230	24.230	0	-292.355	-266.574	195.401
300	21.970	24.360	24.230	.040	-292.352	-266.411	194.078
400	24.200	30.980	25.105	2.350	-292.122	-257.791	140.849
500	26.200	36.600	26.860	4.870	-291.755	-249.252	108.947
600	28.020	41.540	28.907	7.580	-291.286	-240.794	87.708
700	29.760	45.990	31.033	10.470	-290.725	-232.426	72.566
720	30.098	46.833	31.460	11.069	-290.605	-230.758	70.044
720	30.098	46.833	31.460	11.069	-290.825	-230.758	70.044
800	31.450	50.070	33.158	13.530	-290.264	-224.109	61.223
900	33.130	53.870	35.248	16.760	-289.505	-215.867	52.419
1000	34.780	57.450	37.300	20.150	-288.747	-207.754	45.404

Phase change: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 18.770 + 16.180x10^{-3}T - 1.660x10^{5}T^{-2}$
$H°-H°_{298} = 18.770x10^{-3}T + 8.090x10^{-6}T^{2} + 1.660x10^{2}T^{-1} - 6.872$

Reaction equations (kcal/mol):

298.15-720 K: $ΔHr° = -293.161 - 0.078x10^{-3}T + 4.606x10^{-6}T^{2} + 125.050T^{-1}$
$ΔGr° = -293.161 + 0.078x10^{-3}TlnT - 4.606x10^{-6}T^{2} + 62.525T^{-1} + 89.401x10^{-3}T$
720-1000 K: $ΔHr° = -294.902 + 3.860x10^{-3}T + 2.233x10^{-6}T^{2} + 64.050T^{-1}$
$ΔGr° = -294.902 - 3.860x10^{-3}TlnT - 2.233x10^{-6}T^{2} + 32.025T^{-1} + 116.079x10^{-3}T$

Sources: Enthalpy of formation from Cubicciotti (106). Low-temperature heat capacities and entropy at 298 K from Kelley (248). High-temperature data are those estimated by Schwitzgebel (440).

$CaSO_4(\alpha)$
α-Calcium Sulfate
[Reaction: $Ca(c,l) + 0.5S_2(g) + 2O_2(g) = CaSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	23.940	26.050	26.050	0	-356.075	-323.531	237.152
300	24.010	26.201	26.051	.045	-356.074	-323.328	235.541
400	26.759	33.559	27.039	2.608	-355.946	-312.429	170.701
500	29.019	39.773	28.979	5.397	-355.676	-301.578	131.818
600	31.279	45.263	31.243	8.412	-355.279	-290.791	105.919
700	33.538	50.255	33.608	11.653	-354.756	-280.088	87.446
720	33.990	51.206	34.084	12.328	-354.638	-277.953	84.369
720	33.990	51.206	34.084	12.328	-354.858	-277.953	84.369
800	35.798	54.881	35.981	15.120	-354.286	-269.436	73.606
900	38.058	59.227	38.325	18.812	-353.473	-258.863	62.860
1000	40.318	63.354	40.623	22.731	-352.599	-248.415	54.290
1100	42.577	67.303	42.870	26.876	-351.607	-238.040	47.294
1112	42.848	67.766	43.136	27.389	-351.480	-236.807	46.541
1112	42.848	67.766	43.136	27.389	-353.520	-236.807	46.541
1200	44.837	71.104	45.065	31.247	-352.168	-227.621	41.455
1300	47.097	74.782	47.210	35.843	-350.439	-217.313	36.533
1400	49.356	78.355	49.308	40.666	-348.503	-207.142	32.336

Phase changes: 720 K, α – β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15–1400 K: $Cp° = 18.604 + 21.826\times10^{-3}T - 1.042\times10^{5}T^{-2}$
$H° - H°_{298} = 18.604\times10^{-3}T + 10.913\times10^{-6}T^{2} + 1.042\times10^{2}T^{-1} - 6.866$

Reaction equations (kcal/mol):

298.15–720 K: $\Delta Hr° = -355.699 - 3.859\times10^{-3}T + 7.177\times10^{-6}T^{2} + 40.650T^{-1}$
$\Delta Gr° = -355.699 + 3.859\times10^{-3}T\ln T - 7.177\times10^{-6}T^{2} + 20.325T^{-1} + 87.819\times10^{-3}T$
720–1112 K: $\Delta Hr° = -357.440 + 0.079\times10^{-3}T + 4.805\times10^{-6}T^{2} - 20.350T^{-1}$
$\Delta Gr° = -357.440 - 0.079\times10^{-3}T\ln T - 4.805\times10^{-6}T^{2} - 10.175T^{-1} + 114.497\times10^{-3}T$
1112–1400 K: $\Delta Hr° = -357.688 - 7.028\times10^{-3}T + 9.747\times10^{-6}T^{2} - 20.350T^{-1}$
$\Delta Gr° = -357.688 + 7.028\times10^{-3}T\ln T - 9.747\times10^{-6}T^{2} - 10.175T^{-1} + 70.367\times10^{-3}T$

Source: Data from DeKock (113).

$CaSO_4(\beta)$
β-Calcium Sulfate
[Reaction: $Ca(c,l) + 0.5S_2(g) + 2O_2(g) = CaSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	23.690	25.720	25.720	0	-355.015	-322.373	236.302
300	23.754	25.871	25.721	.045	-355.014	-322.169	234.697
400	26.759	33.229	26.709	2.608	-354.886	-311.237	170.050
500	29.019	39.443	28.649	5.397	-354.616	-300.353	131.283
600	31.279	44.933	30.913	8.412	-354.219	-289.533	105.461
700	33.538	49.925	33.278	11.653	-353.696	-278.797	87.043
720	33.990	50.876	33.754	12.328	-353.578	-276.655	83.975
720	33.990	50.876	33.754	12.328	-353.798	-276.655	83.975
800	35.798	54.551	35.651	15.120	-353.227	-268.112	73.244
900	38.058	58.897	37.995	18.812	-352.413	-257.506	62.530
1000	40.318	63.024	40.293	22.731	-351.539	-247.025	53.986
1100	42.577	66.973	42.540	26.876	-350.547	-236.617	47.011
1112	42.848	67.436	42.806	27.389	-350.421	-235.381	46.261
1112	42.848	67.436	42.806	27.389	-352.461	-235.381	46.261
1200	44.837	70.774	44.735	31.247	-351.108	-226.165	41.190
1300	47.097	74.452	46.880	35.843	-349.379	-215.824	36.283
1400	49.356	78.025	48.978	40.666	-347.443	-205.620	32.098

Phase changes: 720 K, α − β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K:
$$Cp° = 19.030 + 21.456\times10^{-3}T - 1.544\times10^{5}T^{-2}$$
$$H° - H°_{298} = 19.030\times10^{-3}T + 10.728\times10^{-6}T^{2} + 1.544\times10^{2}T^{-1} - 7.145$$

Reaction equations (kcal/mol):

298.15-720 K:
$$\Delta Hr° = -354.918 - 3.432\times10^{-3}T + 6.992\times10^{-6}T^{2} + 90.850T^{-1}$$
$$\Delta Gr° = -354.918 + 3.432\times10^{-3}T\ln T - 6.992\times10^{-6}T^{2} + 45.425T^{-1} + 91.174\times10^{-3}T$$

720-1112 K:
$$\Delta Hr° = -356.659 + 0.506\times10^{-3}T + 4.620\times10^{-6}T^{2} + 29.850T^{-1}$$
$$\Delta Gr° = -356.659 - 0.506\times10^{-3}T\ln T - 4.620\times10^{-6}T^{2} + 14.925T^{-1} + 117.852\times10^{-3}T$$

1112-1400 K:
$$\Delta Hr° = -356.907 - 6.601\times10^{-3}T + 9.562\times10^{-6}T^{2} + 29.850T^{-1}$$
$$\Delta Gr° = -356.907 + 6.601\times10^{-3}T\ln T - 9.562\times10^{-6}T^{2} + 14.925T^{-1} + 73.723\times10^{-3}T$$

Source: Data from DeKock (113).

$CaSO_4(c)$
Calcium Sulfate, Insoluble Anhydrite
[Reaction: $Ca(c,l) + 0.5S_2(g) + 2O_2(g) = CaSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	23.878	25.620	25.620	0	-358.195	-325.523	238.612
300	23.965	25.771	25.621	.045	-358.194	-325.319	236.991
400	26.759	33.129	26.609	2.608	-358.066	-314.377	171.765
500	29.019	39.343	28.549	5.397	-357.796	-303.483	132.651
600	31.279	44.833	30.813	8.412	-357.398	-292.653	106.597
700	33.538	49.825	33.178	11.653	-356.876	-281.907	88.014
720	33.990	50.776	33.654	12.328	-356.758	-279.763	84.919
720	33.990	50.776	33.654	12.328	-356.978	-279.763	84.919
800	35.798	54.451	35.551	15.120	-356.406	-271.212	74.091
900	38.058	58.797	37.895	18.812	-355.592	-260.596	63.280
1000	40.318	62.924	40.193	22.731	-354.719	-250.105	54.660
1100	42.577	66.873	42.440	26.876	-353.727	-239.687	47.621
1112	42.848	67.336	42.706	27.389	-353.600	-238.449	46.864
1112	42.848	67.336	42.706	27.389	-355.640	-238.449	46.864
1200	44.837	70.674	44.635	31.247	-354.288	-229.225	41.747
1300	47.097	74.352	46.780	35.843	-352.559	-218.874	36.796
1400	49.356	77.925	48.878	40.666	-350.623	-208.660	32.573

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 18.710 + 21.734\times10^{-3}T - 1.166\times10^{5}T^{-2}$
$H°- H°_{298} = 18.710\times10^{-3}T + 10.867\times10^{-6}T^{2} + 1.166\times10^{2}T^{-1} - 6.935$

Reaction equations (kcal/mol):

298.15-720 K: $\Delta Hr° = -357.888 - 3.753\times10^{-3}T + 7.131\times10^{-6}T^{2} + 53.050T^{-1}$
$\Delta Gr° = -357.888 + 3.753\times10^{-3}T\ln T - 7.131\times10^{-6}T^{2} + 26.525T^{-1} + 89.001\times10^{-3}T$
720-1112 K: $\Delta Hr° = -359.629 + 0.185\times10^{-3}T + 4.759\times10^{-6}T^{2} - 7.950T^{-1}$
$\Delta Gr° = -359.629 - 0.185\times10^{-3}T\ln T - 4.759\times10^{-6}T^{2} - 3.975T^{-1} + 115.679\times10^{-3}T$
1112-1400 K: $\Delta Hr° = -359.877 - 6.922\times10^{-3}T + 9.701\times10^{-6}T^{2} - 7.950T^{-1}$
$\Delta Gr° = -359.877 + 6.922\times10^{-3}T\ln T - 9.701\times10^{-6}T^{2} - 3.975T^{-1} + 71.550\times10^{-3}T$

Source: Data from DeKock (113).

$CaSO_4 \cdot 1/2H_2O(\alpha)$
α-Calcium Sulfate Hemihydrate
[Reaction: $Ca(c) + 0.5S_2(g) + 2.25O_2(g) + 0.5H_2(g) = CaSO_4 \cdot 1/2H_2O(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	28.543	31.200	31.200	0	-392.285	-352.972	258.732
300*	28.632	31.377	31.200	.053	-392.286	-352.726	256.957
350	30.745	35.957	31.557	1.540	-392.267	-346.134	216.133
400	32.249	40.167	32.375	3.117	-392.181	-339.549	185.518
450	33.144	44.023	33.456	4.755	-392.055	-332.977	161.714
500	33.429	47.536	34.694	6.421	-391.928	-326.421	142.677
550	33.105	50.711	36.007	8.087	-391.827	-319.873	127.104

*Data above 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 41.154 - 8.410 \times 10^{-3}T - 8.981 \times 10^{5}T^{-2}$
$H° - H°_{298} = 41.154 \times 10^{-3}T - 4.205 \times 10^{-6}T^{2} + 8.981 \times 10^{2}T^{-1} - 14.909$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -398.410 + 13.656 \times 10^{-3}T - 8.276 \times 10^{-6}T^{2} + 831.500T^{-1}$
$\Delta Gr° = -398.410 - 13.656 \times 10^{-3}T\ln T + 8.276 \times 10^{-6}T^{2} + 415.750T^{-1} + 223.062 \times 10^{-3}T$

Source: Data from DeKock (113) who estimated all above 298 K.

$CaSO_4 \cdot 1/2H_2O(\beta)$
β-Calcium Sulfate Hemihydrate
[Reaction: $Ca(c) + 0.5S_2(g) + 2.25O_2(g) + 0.5H_2(g) = CaSO_4 \cdot 1/2H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	29.690	32.100	32.100	0	-391.785	-352.740	258.562
300*	29.802	32.284	32.101	.055	-391.784	-352.496	256.790
350	32.995	37.119	32.476	1.625	-391.682	-345.956	216.022
400	36.114	41.729	33.347	3.353	-391.445	-339.437	185.458
450	39.159	46.159	34.526	5.235	-391.075	-332.958	161.704
500	42.129	50.439	35.903	7.268	-390.581	-326.525	142.722
550	45.025	54.591	37.415	9.447	-389.967	-320.147	127.213

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 13.537 + 57.980 \times 10^{-3}T - 1.008 \times 10^{5}T^{-2}$

$H°- H°_{298} = 13.537 \times 10^{-3}T + 28.990 \times 10^{-6}T^{2} + 1.008 \times 10^{2}T^{-1} - 6.951$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -389.952 - 13.961 \times 10^{-3}T + 24.919 \times 10^{-6}T^{2} + 34.200T^{-1}$

$\Delta Gr° = -389.952 + 13.961 \times 10^{-3}T\ln T - 24.919 \times 10^{-6}T^{2} + 17.100T^{-1} + 52.504 \times 10^{-3}T$

Source: Data from DeKock (113) who estimated all above 298 K.

$CaSO_4 \cdot 2H_2O(c)$
Calcium Sulfate Dihydrate
[Reaction: $Ca(c) + 0.5S_2(g) + 3O_2(g) + 2H_2(g) = CaSO_4 \cdot 2H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	44.102	46.400	46.400	0	-498.855	-439.159	321.908
300*	44.236	46.673	46.400	.082	-498.856	-438.787	319.652
350	47.157	53.729	46.952	2.372	-498.818	-428.777	267.737
400	48.756	60.145	48.208	4.775	-498.696	-418.779	228.807
450	49.033	65.916	49.858	7.226	-498.553	-408.798	198.537
500	47.988	71.040	51.726	9.657	-498.461	-398.831	174.327
550	45.621	75.513	53.691	12.002	-498.487	-388.867	154.520

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 81.276 - 51.320 \times 10^{-3}T - 19.444 \times 10^{5}T^{-2}$

$H°- H°_{298} = 81.276 \times 10^{-3}T - 25.660 \times 10^{-6}T^{2} + 19.444 \times 10^{2}T^{-1} - 28.473$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -513.920 + 38.671 \times 10^{-3}T - 30.737 \times 10^{-6}T^{2} + 1868.650T^{-1}$

$\Delta Gr° = -513.920 - 38.671 \times 10^{-3}T\ln T + 30.737 \times 10^{-6}T^{2} + 934.325T^{-1} + 451.410 \times 10^{-3}T$

Source: Data from DeKock (113) who estimated all above 298 K.

$CaSiO_3$(wollastonite)
Calcium Silicate, Wollastonite
[Formation: $Ca(c,l) + Si(c) + 1.5O_2(g) = CaSiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	20.663	19.474	19.474	0	-390.690	-370.275	271.415
300	20.732	19.602	19.475	.038	-390.691	-370.147	269.648
400	23.655	25.999	20.326	2.269	-390.648	-363.302	198.496
500	25.588	31.498	22.024	4.737	-390.466	-356.484	155.817
600	26.964	36.292	24.012	7.368	-390.223	-349.709	127.380
700	27.988	40.529	26.075	10.118	-389.964	-342.983	107.083
720	28.145	41.320	26.487	10.679	-389.913	-341.638	103.700
720	28.145	41.320	26.487	10.679	-390.133	-341.638	103.700
800	28.773	44.319	28.122	12.958	-389.892	-336.259	91.860
900	29.387	47.745	30.115	15.867	-389.633	-329.555	80.026
1000	29.873	50.868	32.037	18.831	-389.486	-322.899	70.569
1100	30.259	53.733	33.880	21.838	-389.401	-316.249	62.832
1112	30.296	54.062	34.096	22.201	-389.397	-315.457	61.998
1112	30.296	54.062	34.096	22.201	-391.437	-315.457	61.998
1200	30.567	56.380	35.647	24.880	-391.061	-309.459	56.359
1300	30.812	58.837	37.337	27.950	-390.625	-302.677	50.884
1400	31.004	61.128	38.956	31.041	-390.188	-295.923	46.195
1500	31.151	63.272	40.506	34.149	-389.748	-289.221	42.139

Phase changes: 720 K, α – β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 25.816 + 4.396\times10^{-3}T - 5.747\times10^{5}T^{-2}$
$H°-H°_{298} = 25.816\times10^{-3}T + 2.198\times10^{-6}T^{2} + 5.747\times10^{2}T^{-1} - 9.820$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -393.761 + 5.461\times10^{-3}T - 1.478\times10^{-6}T^{2} + 469.400T^{-1}$
$\Delta Gf° = -393.761 - 5.461\times10^{-3}T\ln T + 1.478\times10^{-6}T^{2} + 234.700T^{-1} + 106.808\times10^{-3}T$
720-1112 K: $\Delta Hf° = -395.502 + 9.399\times10^{-3}T - 3.849\times10^{-6}T^{2} + 408.400T^{-1}$
$\Delta Gf° = -395.502 - 9.399\times10^{-3}T\ln T + 3.849\times10^{-6}T^{2} + 204.200T^{-1} + 133.486\times10^{-3}T$
1112-1500 K: $\Delta Hf° = -395.750 + 2.292\times10^{-3}T + 1.092\times10^{-6}T^{2} + 408.400T^{-1}$
$\Delta Gf° = -395.750 - 2.292\times10^{-3}T\ln T - 1.092\times10^{-6}T^{2} + 204.200T^{-1} + 89.357\times10^{-3}T$

Source: Data from Robinson (428).

$CaSiO_3$(pseudowollastonite)
Calcium Silicate, Pseudowollastonite
[Formation: $Ca(c,l,g) + Si(c,l) + 1.5O_2(g) = CaSiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	21.249	20.859	20.859	0	-389.220	-369.218	270.640
300	21.307	20.991	20.861	.039	-389.220	-369.093	268.880
400	23.685	27.478	21.728	2.300	-389.148	-362.393	198.000
500	25.168	32.933	23.439	4.747	-388.986	-355.722	155.484
600	26.206	37.619	25.421	7.319	-388.802	-349.085	127.152
700	26.984	41.719	27.462	9.980	-388.632	-342.484	106.927
720	27.107	42.481	27.869	10.521	-388.602	-341.163	103.556
720	27.107	42.481	27.869	10.521	-388.822	-341.163	103.556
800	27.597	45.364	29.476	12.710	-388.670	-335.873	91.755
900	28.095	48.644	31.426	15.496	-388.534	-329.265	79.956
1000	28.511	51.626	33.300	18.326	-388.521	-322.692	70.523
1100	28.866	54.361	35.092	21.196	-388.574	-316.112	62.805
1112	28.903	54.674	35.302	21.543	-388.586	-315.327	61.973
1112	28.903	54.674	35.302	21.543	-390.626	-315.327	61.973
1200	29.172	56.886	36.804	24.098	-390.374	-309.378	56.345
1300	29.441	59.232	38.440	27.029	-390.077	-302.642	50.878
1400	29.679	61.423	40.005	29.985	-389.774	-295.922	46.195
1500	29.891	63.478	41.502	32.964	-389.463	-289.245	42.142
1600	30.083	65.413	42.936	35.963	-389.147	-282.578	38.598
1687	30.234	67.010	44.137	38.587	-388.869	-276.760	35.854
1687	30.234	67.010	44.137	38.587	-400.951	-276.760	35.854
1700	30.257	67.242	44.313	38.980	-400.900	-275.799	35.456
1757	30.348	68.241	45.073	40.708	-400.677	-271.606	33.784
1757	30.348	68.241	45.073	40.708	-437.303	-271.606	33.784
1800	30.416	68.976	45.635	42.014	-437.048	-267.520	32.481

Phase changes: 720 K, α − β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal.mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 25.841 + 2.926\times10^{-3}T - 4.857\times10^{5}T^{-2}$
$H° - H°_{298} = 25.841\times10^{-3}T + 1.463\times10^{-6}T^{2} + 4.857\times10^{2}T^{-1} - 9.464$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -391.935 + 5.486\times10^{-3}T - 2.213\times10^{-6}T^{2} + 380.400T^{-1}$
$\Delta Gf° = -391.935 - 5.486\times10^{-3}T\ln T + 2.213\times10^{-6}T^{2} + 190.200T^{-1} + 104.652\times10^{-3}T$
720-1112 K: $\Delta Hf° = -393.676 + 9.424\times10^{-3}T - 4.584\times10^{-6}T^{2} + 319.400T^{-1}$
$\Delta Gf° = -393.676 - 9.424\times10^{-3}T\ln T + 4.584\times10^{-6}T^{2} + 159.700T^{-1} + 131.330\times10^{-3}T$
1112-1687 K: $\Delta Hf° = -393.924 + 2.317\times10^{-3}T + 0.357\times10^{-6}T^{2} + 319.400T^{-1}$
$\Delta Gf° = -393.924 - 2.317\times10^{-3}T\ln T - 0.357\times10^{-6}T^{2} + 159.700T^{-1} + 87.201\times10^{-3}T$
1687-1757 K: $\Delta Hf° = -406.353 + 1.896\times10^{-3}T + 0.709\times10^{-6}T^{2} + 417.900T^{-1}$
$\Delta Gf° = -406.353 - 1.896\times10^{-3}T\ln T - 0.709\times10^{-6}T^{2} + 208.950T^{-1} + 92.015\times10^{-3}T$
1757-1800 K: $\Delta Hf° = -446.524 + 3.926\times10^{-3}T + 0.701\times10^{-6}T^{2} + 417.900T^{-1}$
$\Delta Gf° = -446.524 - 3.926\times10^{-3}T\ln T - 0.701\times10^{-6}T^{2} + 208.950T^{-1} + 130.033\times10^{-3}T$

Source: Data from Robinson (428).

$Ca_2SiO_4(c)$
Dicalcium Silicate
[Formation: $2Ca(c,l,g) + Si(c,l) + 2O_2(g) = Ca_2SiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	30.310	28.850	28.850	0	-554.000	-526.111	385.645
300	30.400	29.037	28.850	.056	-554.001	-525.936	383.139
400	33.745	38.255	30.083	3.269	-553.947	-516.585	282.245
500	36.143	46.055	32.517	6.769	-553.741	-507.268	221.724
600	38.045	52.819	35.351	10.481	-553.479	-497.994	181.392
700	39.666	58.808	38.282	14.368	-553.203	-488.779	152.602
720	39.953	59.929	38.868	15.164	-553.151	-486.932	147.802
720	39.953	59.929	38.868	15.164	-553.591	-486.932	147.802
800	41.099	64.200	41.190	18.408	-553.296	-479.536	131.001
900	42.384	69.116	44.024	22.583	-552.989	-470.304	114.204
1000	43.546	73.643	46.762	26.881	-552.869	-461.152	100.783
1100	44.598	77.843	49.398	31.289	-552.830	-451.985	89.800
1112	44.715	78.321	49.710	31.816	-552.842	-450.898	88.617
1112	44.715	78.321	49.710	31.816	-556.922	-450.898	88.617
1121	44.803	78.682	49.941	32.219	-556.855	-450.034	87.737
1121	43.986	81.753	49.941	35.662	-553.412	-450.034	87.737
1200	44.956	84.789	52.136	39.184	-552.847	-442.775	80.639
1300	46.180	88.436	54.789	43.741	-552.052	-433.635	72.900
1400	47.404	91.903	57.317	48.420	-551.158	-424.552	66.275
1500	48.628	95.215	59.734	53.222	-550.159	-415.562	60.547
1600	49.851	98.392	62.051	58.146	-549.057	-406.631	55.543
1687	50.916	101.060	63.994	62.529	-548.012	-398.874	51.673
1687	50.916	101.060	63.994	62.529	-560.094	-398.874	51.673
1700	51.075	101.451	64.279	63.192	-559.922	-397.628	51.118
1712	51.223	101.813	64.542	63.809	-559.759	-396.484	50.614
1712	48.908	103.794	64.542	67.200	-556.368	-396.484	50.614
1757	48.908	105.060	65.563	69.397	-555.874	-392.287	48.795
1757	48.908	105.060	65.563	69.397	-629.126	-392.287	48.795
1800	48.908	106.243	66.521	71.500	-628.480	-386.432	46.919

Phase changes:
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1121 K, γ - α' transition point of Ca_2SiO_4; ΔH° = 3.443 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal.mol.
1712 K, α' - α transition point of Ca_2SiO_4; ΔH° = 3.391 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1121 K: $Cp° = 31.893 + 12.190\times10^{-3}T - 4.638\times10^{5}T^{-2}$
$H°-H°_{298} = 31.893\times10^{-3}T + 6.095\times10^{-6}T^{2} + 4.638\times10^{2}T^{-1} - 11.606$
1121-1712 K: $Cp° = 31.653 + 11.572\times10^{-3}T - 8.026\times10^{5}T^{-2}$
$H°-H°_{298} = 31.653\times10^{-3}T + 5.786\times10^{-6}T^{2} + 8.026\times10^{2}T^{-1} - 7.808$
1712-1800 K: $Cp° = 48.907$
$H°-H°_{298} = 48.907\times10^{-3}T - 16.529$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -556.516 + 4.092\times10^{-3}T - 0.402\times10^{-6}T^{2} + 396.900T^{-1}$
$\Delta Gf° = -556.516 - 4.092\times10^{-3}T\ln T + 0.402\times10^{-6}T^{2} + 198.450T^{-1} + 122.940\times10^{-3}T$
720-1112 K: $\Delta Hf° = -559.998 + 11.968\times10^{-3}T - 5.146\times10^{-6}T^{2} + 274.900T^{-1}$
$\Delta Gf° = -559.998 - 11.968\times10^{-3}T\ln T + 5.146\times10^{-6}T^{2} + 137.450T^{-1} + 176.296\times10^{-3}T$
1112-1121 K: $\Delta Hf° = -560.494 - 2.246\times10^{-3}T + 4.738\times10^{-6}T^{2} + 274.900T^{-1}$
$\Delta Gf° = -560.494 + 2.246\times10^{-3}T\ln T - 4.738\times10^{-6}T^{2} + 137.450T^{-1} + 88.037\times10^{-3}T$
1121-1687 K: $\Delta Hf° = -556.696 - 2.486\times10^{-3}T + 4.429\times10^{-6}T^{2} + 613.700T^{-1}$
$\Delta Gf° = -556.696 + 2.486\times10^{-3}T\ln T - 4.429\times10^{-6}T^{2} + 306.850T^{-1} + 82.483\times10^{-3}T$
1687-1712 K: $\Delta Hf° = -569.125 - 2.907\times10^{-3}T + 4.780\times10^{-6}T^{2} + 712.200T^{-1}$
$\Delta Gf° = -569.125 + 2.907\times10^{-3}T\ln T - 4.780\times10^{-6}T^{2} + 356.100T^{-1} + 87.297\times10^{-3}T$
1712-1757 K: $\Delta Hf° = -577.845 + 14.347\times10^{-3}T - 1.006\times10^{-6}T^{2} - 90.400T^{-1}$
$\Delta Gf° = -577.845 - 14.347\times10^{-3}T\ln T + 1.006\times10^{-6}T^{2} - 45.200T^{-1} + 211.085\times10^{-3}T$
1757-1800 K: $\Delta Hf° = -658.188 + 18.407\times10^{-3}T - 1.020\times10^{-6}T^{2} - 90.400T^{-1}$
$\Delta Gf° = -658.188 - 18.407\times10^{-3}T\ln T + 1.020\times10^{-6}T^{2} - 45.200T^{-1} + 287.121\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from King (263). High-temperature data based on Coughlin (102).

Ca_3SiO_5(c)
Tricalcium Silicate
[Formation: $3Ca(c,l,g) + Si(c,l) + 2.5O_2(g) = Ca_3SiO_5(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	41.014	40.296	40.296	0	-701.040	-666.295	488.401
300	41.133	40.550	40.297	.076	-701.039	-666.076	485.230
400	46.211	53.133	41.978	4.462	-700.783	-654.454	357.572
500	49.625	63.834	45.306	9.264	-700.283	-642.929	281.020
600	52.109	73.112	49.185	14.356	-699.702	-631.506	230.023
700	54.011	81.294	53.200	19.666	-699.124	-620.202	193.633
720	54.313	82.820	54.001	20.749	-699.018	-617.938	187.567
720	54.313	82.820	54.001	20.749	-699.678	-617.938	187.567
800	55.521	88.608	57.176	25.146	-699.142	-608.877	166.335
900	56.752	95.221	61.042	30.761	-698.612	-597.582	145.111
1000	57.776	101.255	64.766	36.489	-698.424	-586.414	128.159
1100	58.640	106.803	68.338	42.311	-698.417	-575.215	114.283
1112	58.729	107.440	68.757	43.015	-698.434	-573.887	112.789
1112	58.729	107.440	68.757	43.015	-704.554	-573.887	112.789
1200	59.380	111.938	71.761	48.213	-703.637	-563.583	102.641
1300	60.019	116.717	75.037	54.184	-702.556	-551.957	92.791
1400	60.576	121.185	78.175	60.214	-701.443	-540.405	84.360
1500	61.065	125.382	81.184	66.297	-700.298	-528.968	77.070
1600	61.496	129.337	84.071	72.425	-699.131	-517.594	70.699
1687	61.830	132.602	86.491	77.790	-698.097	-507.700	65.771
1687	61.830	132.602	86.491	77.790	-710.179	-507.700	65.771
1700	61.880	133.077	86.845	78.594	-710.014	-506.136	65.067
1757	62.074	135.121	88.378	82.128	-709.289	-499.312	62.108
1757	62.074	135.121	88.378	82.128	-819.167	-499.312	62.108
1800	62.221	136.624	89.513	84.800	-818.358	-491.395	59.663

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal.mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 50.693 + 7.466\times10^{-3}T - 10.583\times10^{5}T^{-2}$
$H°- H°_{298} = 50.693\times10^{-3}T + 3.733\times10^{-6}T^{2} + 10.583\times10^{2}T^{-1} - 18.996$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Df° = -708.603 + 15.446\times10^{-3}T - 5.586\times10^{-6}T^{2} + 1029.800T^{-1}$
$\Delta Gf° = -708.603 - 15.446\times10^{-3}T\ln T + 5.586\times10^{-6}T^{2} + 514.900T^{-1} + 222.449\times10^{-3}T$
720-1112 K: $\Delta Df° = -713.826 + 27.260\times10^{-3}T - 12.701\times10^{-6}T^{2} + 846.800T^{-1}$
$\Delta Gf° = -713.826 - 27.260\times10^{-3}T\ln T + 12.701\times10^{-6}T^{2} + 423.400T^{-1} + 302.484\times10^{-3}T$
1112-1687 K: $\Delta Df° = -714.570 + 5.939\times10^{-3}T + 2.125\times10^{-6}T^{2} + 846.800T^{-1}$
$\Delta Gf° = -714.570 - 5.939\times10^{-3}T\ln T - 2.125\times10^{-6}T^{2} + 423.400T^{-1} + 170.096\times10^{-3}T$
1687-1757 K: $\Delta Df° = -726.999 + 5.518\times10^{-3}T + 2.476\times10^{-6}T^{2} + 945.300T^{-1}$
$\Delta Gf° = -726.999 - 5.518\times10^{-3}T\ln T - 2.476\times10^{-6}T^{2} + 472.650T^{-1} + 174.910\times10^{-3}T$
1757-1800 K: $\Delta Df° = -847.512 + 11.608\times10^{-3}T + 2.455\times10^{-6}T^{2} + 945.300T^{-1}$
$\Delta Gf° = -847.512 - 11.608\times10^{-3}T\ln T - 2.455\times10^{-6}T^{2} + 472.650T^{-1} + 288.964\times10^{-3}T$

Source: Data from Haas (198).

$Ca_3Si_2O_7(c)$
Tricalcium Disilicate, Rankinite
[Formation: $3Ca(c,l) + 2Si(c) + 3.5O_2(g) = Ca_3Si_2O_7(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	51.235	50.335	50.335	0	-949.600	-901.895	661.099
300	51.390	50.652	50.335	.095	-949.602	-901.596	656.804
400	57.974	66.412	52.440	5.589	-949.454	-885.609	483.868
500	62.235	79.838	56.610	11.614	-949.009	-869.696	380.139
600	65.152	91.458	61.471	17.992	-948.469	-853.879	311.021
700	67.213	101.665	66.499	24.616	-947.946	-838.172	261.686
720	67.508	103.563	67.503	25.963	-947.855	-835.025	253.461
720	67.508	103.563	67.503	25.963	-948.515	-835.025	253.461
800	68.688	110.742	71.473	31.415	-948.049	-822.434	224.676
900	69.743	118.897	76.298	38.339	-947.643	-806.713	195.894
1000	70.484	126.286	80.933	45.353	-947.624	-791.095	172.891
1100	70.984	133.029	85.367	52.428	-947.841	-775.442	154.064
1112	71.021	133.799	85.886	53.280	-947.887	-773.577	152.035
1112	71.021	133.799	85.886	53.280	-954.007	-773.577	152.035
1200	71.292	139.219	89.600	59.543	-953.340	-759.325	138.290
1300	71.447	144.933	93.640	66.681	-952.598	-743.190	124.940
1400	71.477	150.229	97.494	73.829	-951.888	-727.094	113.503

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 64.411 + 7.074\times10^{-3}T - 13.587\times10^{5}T^{-2}$
$H - H°_{298} = 64.411\times10^{-3}T + 3.537\times10^{-6}T^{2} + 13.587\times10^{2}T^{-1} - 24.076$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -957.836 + 16.255\times10^{-3}T - 6.635\times10^{-6}T^{2} + 1186.500T^{-1}$
$\Delta Gf° = -957.836 - 16.255\times10^{-3}T\ln T + 6.635\times10^{-6}T^{2} + 593.250T^{-1} + 271.589\times10^{-3}T$
720-1112 K: $\Delta Hf° = -963.059 + 28.069\times10^{-3}T - 13.752\times10^{-6}T^{2} + 1003.500T^{-1}$
$\Delta Gf° = -963.059 - 28.069\times10^{-3}T\ln T + 13.752\times10^{-6}T^{2} + 501.750T^{-1} + 351.623\times10^{-3}T$
1112-1400 K: $\Delta Hf° = -963.803 + 6.748\times10^{-3}T + 1.074\times10^{-6}T^{2} + 1003.500T^{-1}$
$\Delta Gf° = -963.803 - 6.748\times10^{-3}T\ln T - 1.074\times10^{-6}T^{2} + 501.750T^{-1} + 219.235\times10^{-3}T$

Source: Data from Haas (198).

$CaTiO_3(c)$
Calcium Titanate, Perovskite
[Formation: $Ca(c,l,g) + Ti(c) + 1.5O_2(g) = CaTiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	23.340	22.380	22.380	0	-396.900	-376.510	275.986
300	23.440	22.530	22.397	.040	-396.901	-376.386	274.194
400	26.910	29.820	23.345	2.590	-396.648	-369.570	201.921
500	28.490	36.020	25.280	5.370	-396.251	-362.850	158.600
600	29.370	41.290	27.523	8.260	-395.841	-356.208	129.747
700	29.930	45.870	29.827	11.230	-395.459	-349.635	109.159
720	30.012	46.714	30.285	11.829	-395.392	-348.323	105.729
720	30.012	46.714	30.285	11.829	-395.612	-348.323	105.729
800	30.340	49.890	32.077	14.250	-395.315	-343.075	93.723
900	30.690	53.480	34.258	17.300	-395.035	-336.545	81.723
1000	31.000	56.730	36.350	20.380	-394.901	-330.076	72.137
1100	31.310	59.700	38.336	23.500	-394.849	-323.597	64.292
1112	31.348	60.040	38.569	23.876	-394.851	-322.825	63.446
1112	31.348	60.040	38.569	23.876	-396.891	-322.825	63.446
1156	31.489	61.261	39.417	25.251	-396.735	-319.904	60.479
1156	31.489	61.261	39.417	25.251	-397.752	-319.904	60.479
1200	31.630	62.440	40.240	26.640	-397.543	-316.944	57.723
1300	31.960	64.990	42.052	29.820	-397.067	-310.254	52.158
1400	32.320	67.370	43.770	33.040	-396.585	-303.585	47.391
1500	32.710	69.610	45.417	36.290	-396.099	-296.959	43.266
1530	32.830	70.260	45.899	37.270	-395.955	-294.981	42.135
1530	32.030	70.610	45.899	37.810	-395.415	-294.981	42.135
1600	32.030	72.050	47.019	40.050	-395.137	-290.407	39.667
1700	32.030	73.990	48.549	43.250	-394.766	-283.861	36.492
1757	32.030	75.046	49.387	45.083	-394.563	-280.139	34.846
1757	32.030	75.046	49.387	45.083	-431.189	-280.139	34.846
1800	32.030	75.820	50.009	46.460	-430.964	-276.412	33.561

Phase changes:
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1530 K, α - β transition point of $CaTiO_3$; ΔH° = 0.540 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1530 K: $Cp° = 30.039 + 1.778\text{x}10^{-3}T - 6.428\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 30.039\text{x}10^{-3}T + 0.889\text{x}10^{-6}T^{2} + 6.428\text{x}10^{2}T^{-1} - 11.191$
1530-1800 K: $Cp° = 32.030$
$H°-H°_{298} = 32.030\text{x}10^{-3}T - 11.196$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -401.615 + 9.886\text{x}10^{-3}T - 3.559\text{x}10^{-6}T^{2} + 621.200T^{-1}$
$\Delta Gf° = -401.615 - 9.886\text{x}10^{-3}T\ln T + 3.559\text{x}10^{-6}T^{2} + 310.600T^{-1} + 135.972\text{x}10^{-3}T$
720-1112 K: $\Delta Hf° = -403.356 + 13.824\text{x}10^{-3}T - 5.931\text{x}10^{-6}T^{2} + 560.200T^{-1}$
$\Delta Gf° = -403.356 - 13.824\text{x}10^{-3}T\ln T + 5.931\text{x}10^{-6}T^{2} + 280.100T^{-1} + 162.650\text{x}10^{-3}T$
1112-1156 K: $\Delta Hf° = -403.604 + 6.717\text{x}10^{-3}T - 0.988\text{x}10^{-6}T^{2} + 560.200T^{-1}$
$\Delta Gf° = -403.604 - 6.717\text{x}10^{-3}T\ln T + 0.988\text{x}10^{-6}T^{2} + 280.100T^{-1} + 118.521\text{x}10^{-3}T$
1156-1530 K: $\Delta Hf° = -407.641 + 9.117\text{x}10^{-3}T - 1.311\text{x}10^{-6}T^{2} + 1343.100T^{-1}$
$\Delta Gf° = -407.641 - 9.117\text{x}10^{-3}T\ln T + 1.311\text{x}10^{-6}T^{2} + 671.550T^{-1} + 138.273\text{x}10^{-3}T$
1530-1757 K: $\Delta Hf° = -407.646 + 11.108\text{x}10^{-3}T - 2.201\text{x}10^{-6}T^{2} + 700.300T^{-1}$
$\Delta Gf° = -407.646 - 11.108\text{x}10^{-3}T\ln T + 2.201\text{x}10^{-6}T^{2} + 350.150T^{-1} + 151.654\text{x}10^{-3}T$
1757-1800 K: $\Delta Hf° = -447.817 + 13.138\text{x}10^{-3}T - 2.207\text{x}10^{-6}T^{2} + 700.300T^{-1}$
$\Delta Gf° = -447.817 - 13.138\text{x}10^{-3}T\ln T + 2.207\text{x}10^{-6}T^{2} + 350.150T^{-1} + 189.672\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Shomate (452). High-temperature data based on Naylor (353).

$CaTiSiO_5$(c,l)
Calcium Titanium Silicate, Sphene
[Formation: Ca(c,l,g) + Ti(c) + Si(c,l) + $2.5O_2$(g) = $CaTiSiO_5$(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	33.210	30.880	30.880	0	-622.200	-588.392	431.297
300	33.351	31.086	30.880	.062	-622.201	-588.180	428.483
400	38.620	41.516	32.268	3.699	-622.079	-576.851	315.173
500	41.305	50.448	35.034	7.707	-621.730	-565.583	247.213
600	43.022	58.141	38.259	11.929	-621.315	-554.391	201.934
700	44.281	64.871	41.590	16.297	-620.905	-543.268	169.614
720	44.484	66.121	42.254	17.185	-620.827	-541.048	164.228
720	44.484	66.121	42.254	17.185	-621.047	-541.048	164.228
800	45.297	70.852	44.881	20.777	-620.704	-532.177	145.382
900	46.170	76.239	48.071	25.351	-620.333	-521.118	126.543
1000	46.956	81.145	51.137	30.008	-620.077	-510.117	111.485
1100	47.685	85.655	54.072	34.741	-619.888	-499.141	99.169
1112	47.768	86.173	54.416	35.314	-619.872	-497.830	97.841
1112	47.768	86.173	54.416	35.314	-621.912	-497.830	97.841
1156	48.071	88.033	55.660	37.422	-621.678	-492.922	93.189
1156	48.071	88.033	55.660	37.422	-622.695	-492.922	93.189
1200	48.374	89.834	56.881	39.544	-622.411	-487.988	88.874
1300	49.035	93.732	59.567	44.415	-621.751	-476.813	80.159
1400	49.677	97.389	62.139	49.350	-621.074	-465.684	72.696
1500	50.304	100.838	64.605	54.350	-620.372	-454.624	66.238
1600	50.919	104.104	66.972	59.411	-619.653	-443.603	60.593
1670	51.345	106.294	68.576	62.990	-619.138	-435.880	57.042
1670	66.800	124.014	68.576	92.580	-589.548	-435.880	57.042
1687	66.800	124.690	69.139	93.716	-589.160	-434.320	56.265
1687	66.800	124.690	69.139	93.716	-601.242	-434.320	56.265
1700	66.800	125.203	69.565	94.584	-600.938	-433.031	55.669
1757	66.800	127.406	71.406	98.392	-599.613	-427.421	53.165
1757	66.800	127.406	71.406	98.392	-636.239	-427.421	53.165
1800	66.800	129.021	72.763	101.264	-635.164	-422.291	51.272

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1670 K, melting point of $CaTiSiO_5$; ΔH° = 29.590 kcal.mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal.mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1670 K: $Cp^\circ = 42.251 + 5.648\text{x}10^{-3}T - 9.423\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 42.251\text{x}10^{-3}T + 2.824\text{x}10^{-6}T^{2} + 9.423\text{x}10^{2}T^{-1} - 16.009$
1670-1800 K: $Cp^\circ = 66.800$
$H^\circ - H^\circ_{298} = 66.800\text{x}10^{-3}T - 18.976$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -627.326 + 9.189\text{x}10^{-3}T - 2.478\text{x}10^{-6}T^{2} + 777.000T^{-1}$
$\Delta Gf^\circ = -627.326 - 9.189\text{x}10^{-3}T\ln T + 2.478\text{x}10^{-6}T^{2} + 388.500T^{-1} + 177.830\text{x}10^{-3}T$
720-1112 K: $\Delta Hf^\circ = -629.067 + 13.127\text{x}10^{-3}T - 4.849\text{x}10^{-6}T^{2} + 716.000T^{-1}$
$\Delta Gf^\circ = -629.067 - 13.127\text{x}10^{-3}T\ln T + 4.849\text{x}10^{-6}T^{2} + 358.000T^{-1} + 204.508\text{x}10^{-3}T$
1112-1156 K: $\Delta Hf^\circ = -629.315 + 6.020\text{x}10^{-3}T + 0.092\text{x}10^{-6}T^{2} + 716.000T^{-1}$
$\Delta Gf^\circ = -629.315 - 6.020\text{x}10^{-3}T\ln T - 0.092\text{x}10^{-6}T^{2} + 358.000T^{-1} + 160.379\text{x}10^{-3}T$
1156-1670 K: $\Delta Hf^\circ = -633.352 + 8.420\text{x}10^{-3}T - 0.230\text{x}10^{-6}T^{2} + 1498.900T^{-1}$
$\Delta Gf^\circ = -633.352 - 8.420\text{x}10^{-3}T\ln T + 0.230\text{x}10^{-6}T^{2} + 749.450T^{-1} + 180.131\text{x}10^{-3}T$
1670-1687 K: $\Delta Hf^\circ = -636.318 + 32.969\text{x}10^{-3}T - 3.055\text{x}10^{-6}T^{2} + 556.600T^{-1}$
$\Delta Gf^\circ = -636.318 - 32.969\text{x}10^{-3}T\ln T + 3.055\text{x}10^{-6}T^{2} + 278.300T^{-1} + 359.528\text{x}10^{-3}T$
1687-1757 K: $\Delta Hf^\circ = -648.747 + 32.548\text{x}10^{-3}T - 2.704\text{x}10^{-6}T^{2} + 655.100T^{-1}$
$\Delta Gf^\circ = -648.747 - 32.548\text{x}10^{-3}T\ln T + 2.704\text{x}10^{-6}T^{2} + 327.550T^{-1} + 364.342\text{x}10^{-3}T$
1757-1800 K: $\Delta Hf^\circ = -688.918 + 34.578\text{x}10^{-3}T - 2.711\text{x}10^{-6}T^{2} + 655.100T^{-1}$
$\Delta Gf^\circ = -688.918 - 34.578\text{x}10^{-3}T\ln T + 2.711\text{x}10^{-6}T^{2} + 327.550T^{-1} + 402.360\text{x}10^{-3}T$

Sources: Enthalpy of formation from Parker (391). Other data based on King (268).

$CaUO_4(c)$
Calcium Uranate
[Formation: $Ca(c,l) + U(c) + 2O_2(g) = CaUO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	30.966	34.500	34.500	0	-478.400	-452.923	331.997
300	30.987	34.692	34.502	.057	-478.392	-452.764	329.834
400	32.106	43.759	35.729	3.212	-477.959	-444.287	242.744
500	33.225	51.044	38.086	6.479	-477.533	-435.919	190.538
600	34.344	57.200	40.772	9.857	-477.146	-427.631	155.762
700	35.463	62.578	43.511	13.347	-476.812	-419.410	130.944
720	35.687	63.580	44.054	14.058	-476.754	-417.767	126.808
720	35.687	63.580	44.054	14.058	-476.974	-417.767	126.808
800	36.582	67.387	46.200	16.950	-476.724	-411.202	112.334
900	37.701	71.760	48.800	20.664	-476.497	-403.010	97.863
942	38.171	73.490	49.863	22.257	-476.446	-399.583	92.704
942	38.171	73.490	49.863	22.257	-477.113	-399.583	92.704
1000	38.820	75.790	51.300	24.490	-477.008	-394.830	86.289
1025	39.100	76.752	51.909	25.464	-476.955	-392.775	83.746
1025	39.905	76.967	51.909	25.684	-476.735	-392.775	83.746
1049	40.207	77.894	52.493	26.645	-476.665	-390.810	81.421
1049	40.207	77.894	52.493	26.645	-477.802	-390.810	81.421
1100	40.848	79.818	53.716	28.712	-477.597	-386.584	76.806
1112	40.999	80.262	54.000	29.203	-477.548	-385.597	75.783
1112	40.999	80.262	54.000	29.203	-479.588	-385.597	75.783
1200	42.106	83.426	56.043	32.860	-478.846	-378.186	68.876

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1025 K, α - β transition point of $CaUO_4$; ΔH° = 0.220 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1025 K: $Cp° = 27.630 + 11.190\times10^{-3}T$
$H°-H°_{298} = 27.630\times10^{-3}T + 5.595\times10^{-6}T^2 - 8.735$
1025-1200 K: $Cp° = 27.010 + 12.580\times10^{-3}T$
$H°-H°_{298} = 27.010\times10^{-3}T + 6.290\times10^{-6}T^2 - 8.610$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -480.256 + 6.229\times10^{-3}T - 2.203\times10^{-6}T^2 + 58.100T^{-1}$
$\Delta Gf° = -480.256 - 6.229\times10^{-3}T\ln T + 2.203\times10^{-6}T^2 + 29.050T^{-1} + 126.182\times10^{-3}T$
720-942 K: $\Delta Hf° = -481.997 + 10.167\times10^{-3}T - 4.575\times10^{-6}T^2 - 2.900T^{-1}$
$\Delta Gf° = -481.997 - 10.167\times10^{-3}T\ln T + 4.575\times10^{-6}T^2 - 1.450T^{-1} + 152.861\times10^{-3}T$
942-1025 K: $\Delta Hf° = -479.587 + 3.022\times10^{-3}T - 0.353\times10^{-6}T^2 - 90.400T^{-1}$
$\Delta Gf° = -479.587 - 3.022\times10^{-3}T\ln T + 0.353\times10^{-6}T^2 - 45.200T^{-1} + 105.400\times10^{-3}T$
1025-1049 K: $\Delta Hf° = -479.462 + 2.402\times10^{-3}T + 0.342\times10^{-6}T^2 - 90.400T^{-1}$
$\Delta Gf° = -479.462 - 2.402\times10^{-3}T\ln T - 0.342\times10^{-6}T^2 - 45.200T^{-1} + 101.692\times10^{-3}T$
1049-1112 K: $\Delta Hf° = -481.758 + 3.507\times10^{-3}T + 0.342\times10^{-6}T^2 - 90.400T^{-1}$
$\Delta Gf° = -481.758 - 3.507\times10^{-3}T\ln T - 0.342\times10^{-6}T^2 - 45.200T^{-1} + 111.566\times10^{-3}T$
1112-1200 K: $\Delta Hf° = -482.006 - 3.600\times10^{-3}T + 5.284\times10^{-6}T^2 - 90.400T^{-1}$
$\Delta Gf° = -482.006 + 3.600\times10^{-3}T\ln T - 5.284\times10^{-6}T^2 - 45.200T^{-1} + 67.437\times10^{-3}T$

Source: Data from Cordfunke (99).

$CaV_2O_6(c)$
Calcium Vanadate
[Formation: $Ca(c) + 2V(c) + 3O_2(g) = CaV_2O_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	39.860	42.800	42.800	0	-556.700	-518.541	380.096
300*	39.980	43.050	42.803	.074	-556.698	-518.304	377.579
400	44.680	55.260	44.432	4.331	-556.413	-505.539	276.210
500	47.430	65.550	47.658	8.946	-555.906	-492.879	215.434
600	49.360	74.380	51.395	13.791	-555.310	-480.325	174.956
700	50.930	82.110	55.243	18.807	-554.688	-467.884	146.078
720	51.222	83.549	56.009	19.829	-554.563	-465.402	141.267
720	51.222	83.549	56.009	19.829	-554.783	-465.402	141.267
800	52.390	89.000	59.033	23.974	-554.235	-455.494	124.434
900	53.870	95.260	62.720	29.286	-553.561	-443.179	107.617
1000	55.440	101.010	66.259	34.751	-552.947	-430.961	94.185

*Data above 298 K estimated.

Phase change: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 44.764 + 11.090\times10^{-3}T - 7.298\times10^{5}T^{-2}$

$H°- H°_{298} = 44.764\times10^{-3}T + 5.545\times10^{-6}T^{2} + 7.298\times10^{2}T^{-1} - 16.287$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -561.625 + 9.021\times10^{-3}T - 0.758\times10^{-6}T^{2} + 686.600T^{-1}$

$\Delta Gf° = -561.625 - 9.021\times10^{-3}T\ln T + 0.758\times10^{-6}T^{2} + 343.300T^{-1} + 191.814\times10^{-3}T$

720-1000 K: $\Delta Hf° = -563.366 + 12.959\times10^{-3}T - 3.130\times10^{-6}T^{2} + 625.600T^{-1}$

$\Delta Gf° = -563.366 - 12.959\times10^{-3}T\ln T + 3.130\times10^{-6}T^{2} + 312.800T^{-1} + 218.492\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from King (266). Low-temperature heat capacities and entropy at 298 K from King (272). High-temperature data estimated.

$Ca_2V_2O_7$(c)
Dicalcium Vanadate
[Formation: $2Ca(c) + 2V(c) + 3.5O_2(g) = Ca_2V_2O_7(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	50.080	52.700	52.700	0	-736.900	-691.424	506.821
300*	50.230	53.010	52.700	.093	-736.896	-691.139	503.488
400	55.940	68.330	54.753	5.431	-736.501	-675.937	369.310
500	59.260	81.190	58.784	11.203	-735.846	-660.868	288.862
600	61.550	92.210	63.462	17.249	-735.110	-645.936	235.279
700	63.380	101.840	68.271	23.498	-734.377	-631.145	197.050
720	63.714	103.630	69.229	24.769	-734.235	-628.190	190.679
720	63.714	103.630	69.229	24.769	-734.675	-628.190	190.679
800	65.050	110.410	73.010	29.920	-734.034	-616.389	168.387
900	66.710	118.170	77.606	36.508	-733.301	-601.697	146.110
1000	68.470	125.290	82.024	43.266	-732.755	-587.144	128.319

*Data above 298 K estimated.

Phase change: 720 K, α – β transition point of Ca; ΔH° = 0.220 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 56.683 + 12.374\times10^{-3}T - 9.149\times10^{5}T^{-2}$

$H°-H°_{298} = 56.683\times10^{-3}T + 6.187\times10^{-6}T^{2} + 9.149\times10^{2}T^{-1} - 20.519$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -743.715 + 13.494\times10^{-3}T - 2.938\times10^{-6}T^{2} + 910.100T^{-1}$

$\Delta Gf° = -743.715 - 13.494\times10^{-3}T\ln T + 2.938\times10^{-6}T^{2} + 455.050T^{-1} + 246.272\times10^{-3}T$

720-1000 K: $\Delta Hf° = -747.197 + 21.370\times10^{-3}T - 7.682\times10^{-6}T^{2} + 788.100T^{-1}$

$\Delta Gf° = -747.197 - 21.370\times10^{-3}T\ln T + 7.682\times10^{-6}T^{2} + 394.050T^{-1} + 299.629\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from King (266). Low-temperature heat capacities and entropy at 298 K from King (272). High-temperature data estimated.

$Ca_3V_2O_8(c)$
Tricalcium Vanadate
[Formation: $3Ca(c) + 2V(c) + 4O_2(g) = Ca_3V_2O_8(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	60.290	65.700	65.700	0	-902.900	-851.031	623.814
300*	60.460	66.070	65.700	.112	-902.895	-850.704	619.729
400	67.200	84.490	68.165	6.530	-902.391	-833.373	455.328
500	71.180	99.950	73.022	13.464	-901.582	-816.214	356.762
600	73.920	113.180	78.637	20.726	-900.692	-799.213	291.109
700	76.060	124.740	84.414	28.228	-899.826	-782.386	244.269
720	76.434	126.888	85.564	29.753	-899.664	-779.021	236.462
720	76.434	126.888	85.564	29.753	-900.324	-779.021	236.462
800	77.930	135.020	90.110	35.928	-899.570	-765.581	209.144
900	79.710	144.300	95.621	43.811	-898.759	-748.832	181.839
1000	81.510	152.790	100.919	51.871	-898.273	-732.257	160.033

*Data above 298 K estimated.

Phase change: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 68.467 + 14.064\text{x}10^{-3}T - 10.996\text{x}10^{5}T^{-2}$

$H°- H^\circ_{298} = 68.467\text{x}10^{-3}T + 7.032\text{x}10^{-6}T^{2} + 10.996\text{x}10^{2}T^{-1} - 24.727$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -911.581 + 17.832\text{x}10^{-3}T - 4.914\text{x}10^{-6}T^{2} + 1133.200T^{-1}$

$\Delta Gf° = -911.581 - 17.832\text{x}10^{-3}T\ln T + 4.914\text{x}10^{-6}T^{2} + 566.600T^{-1} + 296.845\text{x}10^{-3}T$

720-1000 K: $\Delta Hf° = -916.804 + 29.646\text{x}10^{-3}T - 12.030\text{x}10^{-6}T^{2} + 950.200T^{-1}$

$\Delta Gf° = -916.804 - 29.646\text{x}10^{-3}T\ln T + 12.030\text{x}10^{-6}T^{2} + 475.100T^{-1} + 376.880\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from King (266). Low-temperature heat capacities and entropy at 298 K from King (272). High-temperature data estimated.

$CaWO_4(c)$
Calcium Tungstate
[Formation: $Ca(c,l) + W(c) + 2O_2(g) = CaWO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	27.300	30.210	30.210	0	-393.200	-367.696	269.525
300	27.380	30.380	30.213	.050	-393.198	-367.537	267.747
400	30.490	38.730	31.330	2.960	-392.915	-359.019	196.156
500	32.250	45.740	33.540	6.100	-392.486	-350.600	153.245
600	33.510	51.740	36.073	9.400	-391.998	-342.262	124.667
700	34.560	56.980	38.694	12.800	-391.512	-334.013	104.282
720	34.754	57.956	39.216	13.493	-391.415	-332.367	100.886
720	34.754	57.956	39.216	13.493	-391.635	-332.367	100.886
800	35.530	61.660	41.273	16.310	-391.196	-325.804	89.004
900	36.460	65.900	43.778	19.910	-390.675	-317.642	77.133
1000	37.400	69.790	46.190	23.600	-390.232	-309.572	67.656
1100	38.350	73.400	48.500	27.390	-389.800	-301.514	59.905
1112	38.468	73.817	48.771	27.851	-389.751	-300.557	59.070
1112	38.468	73.817	48.771	27.851	-391.791	-300.557	59.070
1200	39.330	76.780	50.722	31.270	-391.064	-293.377	53.431
1300	40.340	79.960	52.845	35.250	-390.165	-285.260	47.956

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 30.012 + 7.930\times10^{-3}T - 4.513\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 30.012\times10^{-3}T + 3.965\times10^{-6}T^2 + 4.513\times10^{2}T^{-1} - 10.814$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -396.307 + 5.906\times10^{-3}T + 0.018\times10^{-6}T^2 + 400.900T^{-1}$
$\Delta Gf^\circ = -396.307 - 5.906\times10^{-3}T\ln T - 0.018\times10^{-6}T^2 + 200.450T^{-1} + 127.362\times10^{-3}T$
720-1112 K: $\Delta Hf^\circ = -398.048 + 9.844\times10^{-3}T - 2.354\times10^{-6}T^2 + 339.900T^{-1}$
$\Delta Gf^\circ = -398.048 - 9.844\times10^{-3}T\ln T + 2.354\times10^{-6}T^2 + 169.950T^{-1} + 154.040\times10^{-3}T$
1112-1300 K: $\Delta Hf^\circ = -398.296 + 2.737\times10^{-3}T + 2.588\times10^{-6}T^2 + 339.900T^{-1}$
$\Delta Gf^\circ = -398.296 - 2.737\times10^{-3}T\ln T - 2.588\times10^{-6}T^2 + 169.950T^{-1} + 109.910\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K based on King (271) and Lyon (313). High-temperature data based on Yakovleva (536).

$CaZrO_3(c)$
Calcium Zirconate
[Formation: $Ca(c,l) + Zr(c) + 1.5O_2(g) = CaZrO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	23.900	23.920	23.920	0	-424.580	-404.053	296.175
300	23.987	24.068	23.921	.044	-424.577	-403.924	294.255
400	27.074	31.449	24.906	2.617	-424.325	-397.073	216.948
500	28.590	37.670	26.854	5.408	-423.941	-390.303	170.599
600	29.478	42.967	29.109	8.315	-423.542	-383.611	139.728
700	30.072	47.559	31.425	11.294	-423.175	-376.991	117.700
720	30.159	48.407	31.885	11.896	-423.109	-375.668	114.029
720	30.159	48.407	31.885	11.896	-423.329	-375.668	114.029
800	30.509	51.604	33.699	14.324	-423.043	-370.388	101.184
900	30.857	55.218	35.892	17.393	-422.759	-363.807	88.343
1000	31.149	58.485	37.991	20.494	-422.622	-357.284	78.083
1100	31.407	61.466	39.991	23.622	-422.573	-350.750	69.687
1112	31.435	61.807	40.225	23.999	-422.575	-349.972	68.782
1112	31.435	61.807	40.225	23.999	-424.615	-349.972	68.782
1136	31.491	62.479	40.688	24.754	-424.527	-348.359	67.018
1136	31.491	62.479	40.688	24.754	-425.478	-348.359	67.018
1200	31.641	64.209	41.897	26.774	-425.152	-344.026	62.655
1300	31.859	66.750	43.712	29.949	-424.648	-337.288	56.703
1400	32.067	69.119	45.443	33.146	-424.150	-330.584	51.606
1500	32.267	71.338	47.096	36.363	-423.656	-323.922	47.195

Phase changes:
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K:
$Cp° = 30.228 + 1.530\times10^{-3}T - 6.031\times10^{5}T^{-2}$
$H°-H°_{298} = 30.228\times10^{-3}T + 0.765\times10^{-6}T^{2} + 6.031\times10^{2}T^{-1} - 11.103$

Formation equations (kcal/mol):

298.15-720 K:
$\Delta Hf° = -429.008 + 9.559\times10^{-3}T - 3.502\times10^{-6}T^{2} + 563.400T^{-1}$
$\Delta Gf° = -429.008 - 9.559\times10^{-3}T\ln T + 3.502\times10^{-6}T^{2} + 281.700T^{-1} + 133.951\times10^{-3}T$

720-1112 K:
$\Delta Hf° = -430.749 + 13.497\times10^{-3}T - 5.873\times10^{-6}T^{2} + 502.400T^{-1}$
$\Delta Gf° = -430.749 - 13.497\times10^{-3}T\ln T + 5.873\times10^{-6}T^{2} + 251.200T^{-1} + 160.629\times10^{-3}T$

1112-1136 K:
$\Delta Hf° = -430.997 + 6.390\times10^{-3}T - 0.932\times10^{-6}T^{2} + 502.400T^{-1}$
$\Delta Gf° = -430.997 - 6.390\times10^{-3}T\ln T + 0.932\times10^{-6}T^{2} + 251.200T^{-1} + 116.500\times10^{-3}T$

1136-1500 K:
$\Delta Hf° = -433.493 + 7.559\times10^{-3}T - 0.801\times10^{-6}T^{2} + 556.900T^{-1}$
$\Delta Gf° = -433.493 - 7.559\times10^{-3}T\ln T + 0.801\times10^{-6}T^{2} + 278.450T^{-1} + 127.049\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Brown (61). Low-temperature heat capacities and entropy at 298 K from King (270). High-temperature data based on Gvelesiani (197).

$Cd_3As_2(c)$
Tricadmium Diarsenide
[Formation: $3Cd(c) + 2As(\alpha) = Cd_3As_2(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	29.950	49.500	49.500	0	-10.000	-8.596	6.301
300	29.970	49.690	49.507	.055	-10.000	-8.587	6.256
350	30.610	54.360	49.874	1.570	-10.025	-8.355	5.217
400	31.050	58.470	50.683	3.115	-10.045	-8.109	4.430
450	31.430	62.150	51.761	4.675	-10.080	-7.867	3.821
500	32.140	65.490	52.970	6.260	-10.118	-7.619	3.330
507	45.000	65.980	53.150	6.505	-10.102	-7.586	3.270
550	32.850	68.660	54.260	7.920	-10.103	-7.374	2.930

Phase change: 507 K, second order transition of Cd_3As_2; $\Delta H^\circ = 0$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-507 K: $Cp^\circ = 24.631 + 14.910\times10^{-3}T + 0.777\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.631\times10^{-3}T + 7.455\times10^{-6}T^2 - 0.777\times10^{2}T^{-1} - 7.746$

507-550 K: $Cp^\circ = -116.425 + 282.558\times10^{-3}T$

$H^\circ - H^\circ_{298} = -116.425\times10^{-3}T + 141.279\times10^{-6}T^2 + 29.217$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf^\circ = -9.040 - 2.708\times10^{-3}T + 1.975\times10^{-6}T^2 - 97.700T^{-1}$

$\Delta Gf^\circ = -9.040 + 2.708\times10^{-3}T\ln T - 1.975\times10^{-6}T^2 - 48.850T^{-1} - 12.801\times10^{-3}T$

507-550 K: $\Delta Hf^\circ = 27.922 - 143.764\times10^{-3}T + 135.799\times10^{-6}T^2 - 20.000T^{-1}$

$\Delta Gf^\circ = 27.922 + 143.764\times10^{-3}T\ln T - 135.799\times10^{-6}T^2 - 10.000T^{-1} - 896.577\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Entropy at 298 K from Sirota (463). Low-temperature heat capacities from Demidenko (116). High-temperature data based on Lazarev (297).

$CdCO_3(c)$
Cadmium Carbonate, Octavite
[Formation: $Cd(c,l) + C(c) + 1.5O_2(g) = CdCO_3(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.690	22.100	22.100	0	-181.410	-161.983	118.735
300	19.990	22.220	22.100	.040	-181.405	-161.857	117.911
400	22.900	28.340	22.915	2.170	-181.219	-155.371	84.890
500	26.050	33.780	24.540	4.620	-180.846	-148.942	65.102
594.26	29.019	38.530	26.393	7.213	-180.324	-142.974	52.581
594.26	29.019	38.530	26.393	7.213	-181.804	-142.974	52.581
600	29.200	38.810	26.510	7.380	-181.768	-142.595	51.939
700	32.350	43.550	28.607	10.460	-180.990	-136.126	42.500

Phase change: 594.26 K, melting point of Cd; ΔH° = 1.480 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 10.436 + 31.316 \times 10^{-3}T - 0.074 \times 10^{5}T^{-2}$

$H°- H°_{298} = 10.436 \times 10^{-3}T + 15.658 \times 10^{-6}T^{2} + 0.074 \times 10^{2}T^{-1} - 4.528$

Formation equations (kcal/mol):

298.15-594.26 K: $\Delta Hf° = -179.006 - 9.246 \times 10^{-3}T + 12.692 \times 10^{-6}T^{2} - 231.100T^{-1}$

$\Delta Gf° = -179.006 + 9.246 \times 10^{-3}T\ln T - 12.692 \times 10^{-6}T^{2} - 115.550T^{-1} + 9.502 \times 10^{-3}T$

594.26-700 K: $\Delta Hf° = -179.933 - 11.032 \times 10^{-3}T + 14.138 \times 10^{-6}T^{2} - 232.700T^{-1}$

$\Delta Gf° = -179.933 + 11.032 \times 10^{-3}T\ln T - 14.138 \times 10^{-6}T^{2} - 116.350T^{-1} + 0.515 \times 10^{-3}T$

Source: Data from Chang (74).

$CdO(g)$
Cadmium Monoxide (ideal gas)
[Formation: $Cd(c,l,g) + 0.5O_2(g) = CdO(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°₂₉₈)/T	H°- H°₂₉₈	ΔHf°	ΔGf°	
298.15*	8.090	55.669	55.669	0	30	24.399	-17.885
300	8.090	55.719	55.669	.015	29.997	24.365	-17.750
400	8.400	58.096	55.991	.842	29.835	22.510	-12.299
500	8.570	59.990	56.608	1.691	29.654	20.699	-9.048
594.26	8.674	61.480	57.266	2.504	29.462	19.028	-6.998
594.26	8.674	61.480	57.266	2.504	27.982	19.028	-6.998
600	8.680	61.563	57.306	2.554	27.967	18.946	-6.901
700	8.740	62.906	58.013	3.425	27.738	17.457	-5.450
800	8.790	64.077	58.700	4.302	27.507	16.005	-4.372
900	8.820	65.113	59.355	5.182	27.269	14.585	-3.542
1000	8.840	66.044	59.979	6.065	27.029	13.190	-2.883
1040	8.848	66.391	60.219	6.419	26.932	12.630	-2.654
1040	8.848	66.391	60.219	6.419	3.123	12.630	-2.654
1100	8.860	66.887	60.569	6.950	3.104	13.179	-2.618
1200	8.870	67.659	61.128	7.837	3.071	14.096	-2.567
1300	8.880	68.369	61.658	8.724	3.032	15.017	-2.524
1400	8.890	69.027	62.161	9.612	2.992	15.939	-2.488
1500	8.900	69.641	62.640	10.502	2.949	16.866	-2.457
1600	8.900	70.216	63.096	11.392	2.905	17.794	-2.430
1700	8.900	70.756	63.531	12.282	2.857	18.727	-2.407
1800	8.910	71.264	63.946	13.172	2.806	19.663	-2.387
1900	8.910	71.746	64.344	14.064	2.754	20.600	-2.369
2000	8.910	72.204	64.727	14.955	2.699	21.538	-2.354

*Enthalpy of formation at 298 K estimated.

Phase changes: 594.26 K, melting point of Cd; ΔH° = 1.480 kcal/mol.
1040 K, boiling point of Cd; ΔH° = 23.809 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.805 + 0.084x10^{-3}T - 0.658x10^{5}T^{-2}$
$H°- H°_{298} = 8.805x10^{-3}T + 0.042x10^{-6}T^{2} + 0.658x10^{2}T^{-1} - 2.850$

Formation equations (kcal/mol):

298.15-594.26 K: $\Delta Hf° = 30.035 - 0.129x10^{-3}T - 1.655x10^{-6}T^{2} + 44.800T^{-1}$
$\Delta Gf° = 30.035 + 0.129x10^{-3}T\ln T + 1.655x10^{-6}T^{2} + 22.400T^{-1} - 20.386x10^{-3}T$
594.26-1040 K: $\Delta Hf° = 29.109 - 1.915x10^{-3}T - 0.209x10^{-6}T^{2} + 43.200T^{-1}$
$\Delta Gf° = 29.109 + 1.915x10^{-3}T\ln T + 0.209x10^{-6}T^{2} + 21.600T^{-1} - 29.373x10^{-3}T$
1040-2000 K: $\Delta Hf° = 3.077 + 0.222x10^{-3}T - 0.209x10^{-6}T^{2} + 43.200T^{-1}$
$\Delta Gf° = 3.077 - 0.222x10^{-3}T\ln T + 0.209x10^{-6}T^{2} + 21.600T^{-1} + 10.503x10^{-3}T$

Source: Data from Pedley (396) who estimated enthalpy of formation at 298 K.

$(CdO)_2CdSO_4(c)$
Cadmium Oxysulfate
[Reaction: $3Cd(c,l,g) + 0.5S_2(g) + 3O_2(g) = (CdO)_2CdSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	46.126	58.929	58.929	0	-361.045	-315.583	231.326
300	46.341	59.215	58.929	.086	-361.038	-315.297	229.691
400	53.756	73.610	60.843	5.107	-360.451	-300.130	163.981
500	59.053	86.211	64.683	10.764	-359.392	-285.164	124.643
594.26	62.373	96.711	68.946	16.499	-358.140	-271.280	99.767
594.26	62.373	96.711	68.946	16.499	-362.580	-271.280	99.767
600	62.551	97.311	69.214	16.858	-362.507	-270.384	98.486
700	64.696	107.129	73.945	23.229	-361.030	-255.155	79.662
800	66.012	115.859	78.648	29.769	-359.449	-240.134	65.601
900	67.098	123.696	83.225	36.424	-357.806	-225.307	54.711
1000	68.630	130.838	87.634	43.204	-356.081	-210.670	46.041
1040	69.723	133.551	89.348	45.971	-355.347	-204.895	43.057
1040	69.723	133.551	89.348	45.971	-426.774	-204.895	43.057
1100	71.362	137.495	91.868	50.190	-425.230	-192.136	38.173

Phase changes: 594.26 K, melting point of Cd; ΔH° = 1.480 kcal/mol.
1040 K, boiling point of Cd; ΔH° = 23.809 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp^\circ = 58.534 + 12.000\times10^{-3}T - 14.211\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 58.534\times10^{-3}T + 6.000\times10^{-6}T^{2} + 14.211\times10^{2}T^{-1} - 22.752$

Reaction equations (kcal/mol):

298.15-594.26 K: $\Delta Hr^\circ = -370.241 + 16.715\times10^{-3}T - 0.007\times10^{-6}T^{2} + 1256.150T^{-1}$
$\Delta Gr^\circ = -370.241 - 16.715\times10^{-3}T\ln T + 0.007\times10^{-6}T^{2} + 628.075T^{-1} + 271.494\times10^{-3}T$
594.26-1040 K: $\Delta Hr^\circ = -373.021 + 11.357\times10^{-3}T + 4.331\times10^{-6}T^{2} + 1251.350T^{-1}$
$\Delta Gr^\circ = -373.021 - 11.357\times10^{-3}T\ln T - 4.331\times10^{-6}T^{2} + 625.675T^{-1} + 244.533\times10^{-3}T$
1040-1100 K: $\Delta Hr^\circ = -451.116 + 17.768\times10^{-3}T + 4.331\times10^{-6}T^{2} + 1251.350T^{-1}$
$\Delta Gr^\circ = -451.116 - 17.768\times10^{-3}T\ln T - 4.331\times10^{-6}T^{2} + 625.675T^{-1} + 364.161\times10^{-3}T$

Source: Data from DeKock (113).

$CdSO_4(c)$
Cadmium Sulfate
[Reaction: $Cd(c,l) + 0.5S_2(g) + 2O_2(g) = CdSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	23.806	29.408	29.408	0	-238.455	-206.185	151.136
300*	23.875	29.555	29.408	.044	-238.455	-205.983	150.056
400	26.872	36.832	30.380	2.581	-238.372	-195.168	106.633
500	29.513	43.117	32.311	5.403	-238.090	-184.394	80.598
594.26	31.806	48.409	34.452	8.294	-237.670	-174.307	64.104
594.26	31.806	48.409	34.452	8.294	-239.150	-174.307	64.104
600	31.946	48.715	34.587	8.477	-239.122	-173.676	63.261
700	34.289	53.816	36.975	11.789	-238.507	-162.818	50.833
800	36.600	58.546	39.380	15.333	-237.705	-152.059	41.540

*Data above 298 K estimated.

Phase change: 594.26 K, melting point of Cd; ΔH° = 1.480 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp^\circ = 18.645 + 22.798\times10^{-3}T - 1.454\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.645\times10^{-3}T + 11.399\times10^{-6}T^2 + 1.454\times10^{2}T^{-1} - 7.060$

Reaction equations (kcal/mol):

298.15-594.26 K: $\Delta Hr^\circ = -237.730 - 5.306\times10^{-3}T + 8.787\times10^{-6}T^2 + 22.450T^{-1}$

$\Delta Gr^\circ = -237.730 + 5.306\times10^{-3}T\ln T - 8.787\times10^{-6}T^2 + 11.225T^{-1} + 78.067\times10^{-3}T$

594.26-800 K: $\Delta Hr^\circ = -238.656 - 7.092\times10^{-3}T + 10.233\times10^{-6}T^2 + 20.850T^{-1}$

$\Delta Gr^\circ = -238.656 + 7.092\times10^{-3}T\ln T - 10.233\times10^{-6}T^2 + 10.425T^{-1} + 69.080\times10^{-3}T$

Source: Data from DeKock (113) who estimated all above 298 K.

$CdSO_4 \cdot H_2O(c)$
Cadmium Sulfate Monohydrate
[Reaction: $Cd(c) + 0.5S_2(g) + H_2(g) + 2.5O_2(g) = CdSO_4 \cdot H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	32.167	36.814	36.814	0	-311.695	-265.023	194.265
300*	32.284	37.013	36.814	.060	-311.698	-264.731	192.854
350	35.284	42.220	37.220	1.750	-311.747	-256.901	160.414
400	37.949	47.109	38.154	3.582	-311.680	-249.069	136.083
450	40.278	51.716	39.407	5.539	-311.512	-241.251	117.166
500	42.273	56.066	40.856	7.605	-311.260	-233.456	102.042
550	43.933	60.176	42.429	9.761	-310.942	-225.692	89.681

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 27.988 + 32.402 \times 10^{-3}T - 4.873 \times 10^{5}T^{-2}$

$H°-H°_{298} = 27.988 \times 10^{-3}T + 16.201 \times 10^{-6}T^{2} + 4.873 \times 10^{2}T^{-1} - 11.419$

Reaction equations (kcal/mol):

298.15-550 K: $ΔHr° = -312.246 - 6.033 \times 10^{-3}T + 12.918 \times 10^{-6}T^{2} + 358.250T^{-1}$

$ΔGr° = -312.246 + 6.033 \times 10^{-3}T\ln T - 12.918 \times 10^{-6}T^{2} + 179.125T^{-1} + 125.847 \times 10^{-3}T$

Source: Data from DeKock (113) who estimated all above 298 K.

$CdSO_4 \cdot 8/3H_2O(c)$
Cadmium Sulfate Hydrate
[Reaction: $Cd(c) + 0.5S_2(g) + 2.6667H_2(g) + 3.3333O_2(g) = CdSO_4 \cdot 8/3H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	50.985	54.883	54.883	0	-428.765	-359.798	263.735
300*	51.209	55.199	54.883	.095	-428.766	-359.368	261.796
350	57.141	63.542	55.531	2.804	-428.667	-347.808	217.179
400	62.805	71.545	57.035	5.804	-428.308	-336.278	183.731
450	68.201	79.256	59.078	9.080	-427.706	-324.808	157.746
500	73.330	86.710	61.470	12.620	-426.871	-313.417	136.993
550	78.191	93.929	64.094	16.409	-425.814	-302.121	120.050

*Data above 298 K esitmated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 26.538 + 96.640x10^{-3}T - 3.882x10^{5}T^{-2}$

$H°- H°_{298} = 26.538x10^{-3}T + 48.320x10^{-6}T^{2} + 3.882x10^{2}T^{-1} - 13.510$

Reaction equations (kcal/mol):

298.15-550 K: $ΔHr° = -426.269 - 24.268x10^{-3}T + 43.920x10^{-6}T^{2} + 248.985T^{-1}$

$ΔGr° = -426.269 + 24.268x10^{-3}TlnT - 43.920x10^{-6}T^{2} + 124.493T^{-1} + 96.368x10^{-3}T$

Source: Data from DeKock (113) who estimated all above 298 K.

CdSb(c,l)
Cadmium Antimonide
[Formation: Cd(c,l) + Sb(c,l) = CdSb(c,l)]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.270	23.770	23.770	0	-3.440	-3.592	2.633
300	12.280	23.850	23.783	.020	-3.442	-3.595	2.619
400	12.870	27.450	24.250	1.280	-3.429	-3.641	1.989
500	13.720	30.410	25.210	2.600	-3.400	-3.705	1.619
594.26	14.615	32.849	26.226	3.936	-3.317	-3.769	1.386
594.26	14.615	32.849	26.226	3.936	-4.797	-3.769	1.386
600	14.670	32.990	26.290	4.020	-4.793	-3.755	1.368
700	15.670	35.330	27.416	5.540	-4.642	-3.592	1.121
729	15.960	35.970	27.742	6.000	-4.584	-3.548	1.064
729	16.210	46.400	27.742	13.600	3.016	-3.548	1.064
800	14.880	47.840	29.465	14.700	3.122	-4.198	1.147
900	14.140	49.540	31.607	16.140	3.132	-5.112	1.241

Phase changes: 594.26 K, melting point of Cd; $\Delta H^\circ = 1.480$ kcal/mol.
729 K, melting point of CdSb; $\Delta H^\circ = 7.600$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-729 K: $Cp^\circ = 7.796 + 10.980\text{x}10^{-3}T + 1.066\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 7.796\text{x}10^{-3}T + 5.490\text{x}10^{-6}T^{2} - 1.066\text{x}10^{2}T^{-1} - 2.455$
729-900 K: $Cp^\circ = -14.095 + 19.650\text{x}10^{-3}T + 84.925\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = -14.095\text{x}10^{-3}T + 9.825\text{x}10^{-6}T^{2} - 84.925\text{x}10^{2}T^{-1} + 30.303$

Formation equations (kcal/mol):

298.15-594.26 K: $\Delta Hf^\circ = -2.637 - 2.611\text{x}10^{-3}T + 2.872\text{x}10^{-6}T^{2} - 83.400T^{-1}$
$\Delta Gf^\circ = -2.637 + 2.611\text{x}10^{-3}T\ln T - 2.872\text{x}10^{-6}T^{2} - 41.700T^{-1} - 16.754\text{x}10^{-3}T$
594.26-729 K: $\Delta Hf^\circ = -3.564 - 4.397\text{x}10^{-3}T + 4.318\text{x}10^{-6}T^{2} - 85.000T^{-1}$
$\Delta Gf^\circ = -3.564 + 4.397\text{x}10^{-3}T\ln T - 4.318\text{x}10^{-6}T^{2} - 42.500T^{-1} - 25.741\text{x}10^{-3}T$
729-900 K: $\Delta Hf^\circ = 29.194 - 26.288\text{x}10^{-3}T + 8.653\text{x}10^{-6}T^{2} - 8470.900T^{-1}$
$\Delta Gf^\circ = 29.194 + 26.288\text{x}10^{-3}T\ln T - 8.653\text{x}10^{-6}T^{2} - 4235.450T^{-1} - 203.925\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from Danilenko (107). High-temperature data based on Kubaschewski (287) and Schick (436).

CdSe(c)
Cadmium Selenide
[Reaction: Cd(c,l,g) + $0.5Se_2(g)$ = CdSe(c)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	11.850	22.210	22.210	0	-51.250	-45.505	33.355
300*	11.860	22.280	22.210	.022	-51.248	-45.467	33.122
400	12.080	25.730	22.680	1.220	-51.182	-43.554	23.797
500	12.310	28.450	23.570	2.440	-51.131	-41.653	18.206
594.26	12.517	30.590	24.516	3.609	-51.088	-39.870	14.663
594.26	12.517	30.590	24.516	3.609	-52.568	-39.870	14.663
600	12.530	30.710	24.575	3.681	-52.568	-39.743	14.476
700	12.750	32.660	25.596	4.945	-52.519	-37.613	11.743
800	12.970	34.380	26.591	6.231	-52.447	-35.487	9.694
900	13.200	35.920	27.542	7.540	-52.350	-33.369	8.103
1000	13.420	37.320	28.449	8.871	-52.229	-31.264	6.833
1040	13.508	37.848	28.800	9.410	-52.173	-30.435	6.396
1040	13.508	37.848	28.800	9.410	-75.982	-30.435	6.396
1100	13.640	38.610	29.315	10.224	-75.763	-27.812	5.526
1200	13.870	39.810	30.144	11.599	-75.379	-23.475	4.275
1300	14.090	40.930	30.932	12.997	-74.969	-19.165	3.222
1400	14.310	41.980	31.682	14.417	-74.535	-14.889	2.324
1500	14.540	42.970	32.397	15.860	-74.074	-10.636	1.550

*Data above 298 K estimated.

Phase changes: 594.26 K, melting point of Cd; $\Delta H^\circ = 1.480$ kcal/mol.
1040 K, boiling point of Cd; $\Delta H^\circ = 23.809$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 11.192 + 2.230\times10^{-3}T$
$H^\circ - H^\circ_{298} = 11.192\times10^{-3}T + 1.115\times10^{-6}T^2 - 3.436$

Reaction equations (kcal/mol):

298.15-594.26 K: $\Delta Hr^\circ = -51.301 + 0.541\times10^{-3}T - 0.171\times10^{-6}T^2 - 28.350T^{-1}$
$\Delta Gr^\circ = -51.301 - 0.541\times10^{-3}T\ln T + 0.171\times10^{-6}T^2 - 14.175T^{-1} + 22.632\times10^{-3}T$
594.26-1040 K: $\Delta Hr^\circ = -52.228 - 1.245\times10^{-3}T + 1.275\times10^{-6}T^2 - 29.950T^{-1}$
$\Delta Gr^\circ = -52.228 + 1.245\times10^{-3}T\ln T - 1.275\times10^{-6}T^2 - 14.975T^{-1} + 13.645\times10^{-3}T$
1040-1500 K: $\Delta Hr^\circ = -78.259 + 0.892\times10^{-3}T + 1.275\times10^{-6}T^2 - 29.950T^{-1}$
$\Delta Gr^\circ = -78.259 - 0.892\times10^{-3}T\ln T - 1.275\times10^{-6}T^2 - 14.975T^{-1} + 53.521\times10^{-3}T$

Sources: Entropy at 298 K from Shaulov (442). Other data from Mills (332) who estimated all above 298 K.

$CdSiO_3(c)$
Cadmium Silicate
[Formation: $Cd(c,l) + Si(c) + 1.5O_2(g) = CdSiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	21.170	23.300	23.300	0	-284.200	-264.198	193.660
300*	21.230	23.430	23.300	.040	-284.199	-264.071	192.373
400	23.790	29.920	24.170	2.300	-284.147	-257.373	140.620
500	25.530	35.420	25.880	4.770	-283.983	-250.692	109.576
594.26	26.868	39.951	27.759	7.246	-283.763	-244.436	89.895
594.26	26.868	39.951	27.759	7.246	-285.243	-244.436	89.895
600	26.950	40.210	27.877	7.400	-285.231	-244.037	88.889
700	28.220	44.460	29.946	10.160	-284.939	-237.196	74.055
800	29.410	48.310	32.010	13.040	-284.570	-230.402	62.942
900	30.540	51.840	34.018	16.040	-284.121	-223.652	54.309
1000	31.650	55.110	35.960	19.150	-283.590	-216.945	47.413

*Data above 298 K estimated.

Phase change: 594.26 K, melting point of Cd; ΔH° = 1.480 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 21.653 + 10.310\times10^{-3}T - 3.162\times10^{5}T^{-2}$

$H°-H°_{298} = 21.653\times10^{-3}T + 5.155\times10^{-6}T^{2} + 3.162\times10^{2}T^{-1} - 7.975$

Formation equations (kcal/mol):

298.15-594.26 K: $\Delta Hf° = -284.883 - 0.190\times10^{-3}T + 2.603\times10^{-6}T^{2} + 151.500T^{-1}$

$\Delta Gf° = -284.883 + 0.190\times10^{-3}T\ln T - 2.603\times10^{-6}T^{2} + 75.750T^{-1} + 68.220\times10^{-3}T$

594.26-1000 K: $\Delta Hf° = -285.810 - 1.976\times10^{-3}T + 4.049\times10^{-6}T^{2} + 149.900T^{-1}$

$\Delta Gf° = -285.810 + 1.976\times10^{-3}T\ln T - 4.049\times10^{-6}T^{2} + 74.950T^{-1} + 59.233\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from King (264). High-temperature data estimated.

CdTe(c)
Cadmium Telluride
[Reaction: Cd(c,l) + 0.5Te_2(g) = CdTe(c)]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	11.920	22.800	22.800	0	-43.265	-37.148	27.230
300	11.940	22.870	22.800	.022	-43.262	-37.109	27.034
400	12.730	26.420	23.278	1.257	-43.102	-35.084	19.168
500	13.520	29.350	24.212	2.569	-42.902	-33.104	14.470
594.26	14.265	31.743	25.215	3.879	-42.672	-31.272	11.501
594.26	14.265	31.743	25.215	3.879	-44.152	-31.272	11.501
600	14.310	31.880	25.278	3.961	-44.139	-31.143	11.344
700	15.100	34.150	26.391	5.431	-43.844	-29.007	9.056
800	15.890	36.220	27.494	6.981	-43.477	-26.913	7.352
900	16.680	38.130	28.564	8.609	-43.039	-24.859	6.037
1000	17.470	39.930	29.613	10.317	-42.530	-22.865	4.997

Phase change: 594.26 K, melting point of Cd; ΔH° = 1.480 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 9.613 + 7.852\times10^{-3}T - 0.031\times10^{5}T^{-2}$
$H°-H°_{298} = 9.613\times10^{-3}T + 3.926\times10^{-6}T^{2} + 0.031\times10^{2}T^{-1} - 3.226$

Reaction equations (kcal/mol):

298.15-594.26 K: $\Delta Hr° = -43.433 - 0.006\times10^{-3}T + 2.184\times10^{-6}T^{2} - 7.400T^{-1}$
$\Delta Gr° = -43.433 + 0.006\times10^{-3}T\ln T - 2.184\times10^{-6}T^{2} - 3.700T^{-1} + 21.739\times10^{-3}T$
594.26-1000 K: $\Delta Hr° = -44.359 - 1.792\times10^{-3}T + 3.630\times10^{-6}T^{2} - 9.000T^{-1}$
$\Delta Gr° = -44.359 + 1.792\times10^{-3}T\ln T - 3.630\times10^{-6}T^{2} - 4.500T^{-1} + 12.752\times10^{-3}T$

Source: Data from Mills (332).

$CeB_6(c)$
Cerium Hexaboride
[Formation: $Ce(c,l) + 6B(\beta) = CeB_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	24.691	17.700	17.700	0	-84.000	-81.627	59.833
300	24.838	17.853	17.700	.046	-83.996	-81.606	59.449
400	30.266	25.839	18.752	2.835	-83.769	-80.857	44.177
500	33.160	32.931	20.895	6.018	-83.721	-80.126	35.023
600	35.058	39.154	23.431	9.434	-83.882	-79.408	28.924
700	36.484	44.670	26.079	13.014	-84.174	-78.637	24.551
800	37.660	49.620	28.716	16.723	-84.544	-77.808	21.256
900	38.691	54.117	31.294	20.541	-84.983	-76.943	18.684
999	39.621	58.202	33.760	24.418	-85.471	-76.031	16.633
999	39.621	58.202	33.760	24.418	-86.186	-76.031	16.633
1000	39.630	58.242	33.784	24.458	-86.191	-76.023	16.615
1071	40.255	60.982	35.498	27.294	-86.556	-75.320	15.370
1071	40.255	60.982	35.498	27.294	-87.861	-75.320	15.370
1100	40.510	62.061	36.184	28.465	-88.012	-74.978	14.897
1200	41.350	65.622	38.490	32.559	-88.533	-73.763	13.434
1300	42.162	68.964	40.706	36.735	-89.062	-72.492	12.187
1400	42.953	72.118	42.839	40.991	-89.595	-71.196	11.114
1500	43.729	75.108	44.891	45.325	-90.140	-69.842	10.176
1600	44.493	77.955	46.870	49.736	-90.698	-68.546	9.363
1700	45.248	80.675	48.779	54.223	-91.264	-67.133	8.630
1800	45.997	83.282	50.624	58.785	-91.839	-65.635	7.969
1900	46.739	85.789	52.409	63.422	-92.423	-64.149	7.379
2000	47.478	88.205	54.139	68.133	-93.017	-62.727	6.854

*Data estimated.

Phase changes: 999 K, γ - δ transition point of Ce; ΔH° = 0.715 kcal/mol.
1071 K, melting point of Ce; ΔH° = 1.305 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2463 K: $Cp° = 33.480 + 7.120x10^{-3}T - 9.700x10^{5}T^{-2}$
$H°-H°_{298} = 33.480x10^{-3}T + 3.560x10^{-6}T^{2} + 9.700x10^{2}T^{-1} - 13.552$

Formation equations (kcal/mol):

298.15-999 K: $ΔHf° = -82.645 + 0.057x10^{-3}T - 2.539x10^{-6}T^{2} - 341.800T^{-1}$
$ΔGf° = -82.645 - 0.057x10^{-3}T\ln T + 2.539x10^{-6}T^{2} - 170.900T^{-1} + 4.905x10^{-3}T$
999-1071 K: $ΔHf° = -81.385 - 3.848x10^{-3}T - 0.592x10^{-6}T^{2} - 359.000T^{-1}$
$ΔGf° = -81.385 + 3.848x10^{-3}T\ln T + 0.592x10^{-6}T^{2} - 179.500T^{-1} - 21.373x10^{-3}T$
1071-2000 K: $ΔHf° = -82.668 - 3.868x10^{-3}T - 0.592x10^{-6}T^{2} - 359.000T^{-1}$
$ΔGf° = -82.668 + 3.868x10^{-3}T\ln T + 0.592x10^{-6}T^{2} - 179.500T^{-1} - 20.314x10^{-3}T$

Source: Data are those estimated by Barin (23).

$CeC_2(c)$
Cerium Dicarbide
[Formation: $Ce(c,l) + 2C(c) = CeC_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.581	21.500	21.500	0	-23.200	-23.664	17.346
300	14.616	21.590	21.500	.027	-23.193	-23.667	17.241
400	15.905	25.994	22.091	1.561	-22.807	-23.882	13.048
500	16.620	29.626	23.246	3.190	-22.505	-24.191	10.574
600	17.109	32.701	24.571	4.878	-22.298	-24.544	8.940
700	17.491	35.368	25.928	6.608	-22.180	-24.935	7.785
800	17.816	37.726	27.259	8.374	-22.135	-25.325	6.918
900	18.108	39.841	28.541	10.170	-22.156	-25.728	6.248
999	18.377	41.745	29.756	11.977	-22.226	-26.120	5.714
999	18.377	41.745	29.756	11.977	-22.941	-26.120	5.714
1000	18.380	41.763	29.768	11.995	-22.942	-26.125	5.710
1071	18.563	43.030	30.606	13.307	-23.009	-26.323	5.371
1071	18.563	43.030	30.606	13.307	-24.314	-26.323	5.371
1100	18.638	43.527	30.940	13.846	-24.343	-26.377	5.241
1200	18.887	45.160	32.058	15.722	-24.444	-26.585	4.842
1300	19.130	46.681	33.125	17.623	-24.544	-26.761	4.499
1400	19.368	48.108	34.145	19.548	-24.638	-26.926	4.203
1500	19.602	49.452	35.121	21.497	-24.726	-27.087	3.947

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 999 K, γ - δ transition point of Ce; ΔH° = 0.715 kcal/mol.
1071 K, melting point of Ce; ΔH° = 1.305 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 16.400 + 2.200\times10^{-3}T - 2.200\times10^{5}T^{-2}$
$H°-H°_{298} = 16.400\times10^{-3}T + 1.100\times10^{-6}T^{2} + 2.200\times10^{2}T^{-1} - 5.725$

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf° = -23.904 + 4.279\times10^{-3}T - 2.379\times10^{-6}T^{2} - 107.400T^{-1}$
$\Delta Gf° = -23.904 - 4.279\times10^{-3}T\ln T + 2.379\times10^{-6}T^{2} - 53.700T^{-1} + 25.080\times10^{-3}T$
999-1071 K: $\Delta Hf° = -22.644 + 0.374\times10^{-3}T - 0.432\times10^{-6}T^{2} - 124.600T^{-1}$
$\Delta Gf° = -22.644 - 0.374\times10^{-3}T\ln T + 0.432\times10^{-6}T^{2} - 62.300T^{-1} - 1.198\times10^{-3}T$
1071-1500 K: $\Delta Hf° = -23.927 + 0.354\times10^{-3}T - 0.432\times10^{-6}T^{2} - 124.600T^{-1}$
$\Delta Gf° = -23.927 - 0.354\times10^{-3}T\ln T + 0.432\times10^{-6}T^{2} - 62.300T^{-1} - 0.139\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Baker (15). Other data are those estimated by Barin (23).

$Ce_2C_3(c)$
Dicerium Tricarbide
[Formation: $2Ce(c,l) + 3C(c) = Ce_2C_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	24.700	41.500	41.500	0	-42.200	-43.090	31.585
300	24.772	41.653	41.500	.046	-42.190	-43.095	31.395
400	27.390	49.186	42.509	2.671	-41.617	-43.480	23.756
500	28.755	55.458	44.490	5.484	-41.141	-44.009	19.236
600	29.627	60.783	46.773	8.406	-40.804	-44.609	16.248
700	30.265	65.400	49.111	11.402	-40.608	-45.271	14.134
800	30.780	69.476	51.407	14.455	-40.538	-45.929	12.547
900	31.222	73.127	53.620	17.556	-40.584	-46.609	11.318
999	31.616	76.406	55.719	20.666	-40.725	-47.271	10.341
999	31.616	76.406	55.719	20.666	-42.155	-47.271	10.341
1000	31.620	76.438	55.740	20.698	-42.157	-47.280	10.333
1071	31.881	78.616	57.185	22.953	-42.290	-47.598	9.713
1071	31.881	78.616	57.185	22.953	-44.900	-47.598	9.713
1100	31.988	79.469	57.761	23.879	-44.956	-47.670	9.471
1200	32.337	82.267	59.688	27.095	-45.156	-47.950	8.733
1300	32.671	84.869	61.526	30.346	-45.357	-48.178	8.099
1400	32.995	87.302	63.281	33.629	-45.553	-48.382	7.553
1500	33.312	89.589	64.960	36.944	-45.744	-48.582	7.078

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 999 K, γ - δ transition point of Ce; ΔH° = 0.715 kcal/mol.
1071 K, melting point of Ce; ΔH° = 1.305 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 29.250 + 2.850\text{x}10^{-3}T - 4.800\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 29.250\text{x}10^{-3}T + 1.425\text{x}10^{-6}T^{2} + 4.800\text{x}10^{2}T^{-1} - 10.457$

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf^\circ = -44.310 + 8.526\text{x}10^{-3}T - 4.767\text{x}10^{-6}T^{2} - 2.500T^{-1}$
$\Delta Gf^\circ = -44.310 - 8.526\text{x}10^{-3}T\ln T + 4.767\text{x}10^{-6}T^{2} - 1.250T^{-1} + 51.263\text{x}10^{-3}T$
999-1071 K: $\Delta Hf^\circ = -41.789 + 0.716\text{x}10^{-3}T - 0.873\text{x}10^{-6}T^{2} - 36.900T^{-1}$
$\Delta Gf^\circ = -41.789 - 0.716\text{x}10^{-3}T\ln T + 0.873\text{x}10^{-6}T^{2} - 18.450T^{-1} - 1.294\text{x}10^{-3}T$
1071-1500 K: $\Delta Hf^\circ = -44.357 + 0.676\text{x}10^{-3}T - 0.873\text{x}10^{-6}T^{2} - 36.900T^{-1}$
$\Delta Gf^\circ = -44.357 - 0.676\text{x}10^{-3}T\ln T + 0.873\text{x}10^{-6}T^{2} - 18.450T^{-1} + 0.824\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Baker (15). Other data are those estimated by Barin (23).

CeN(c)
Cerium Nitride
[Formation: Ce(c,l) + $0.5N_2(g)$ = CeN(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	9.646	10.600	10.600	0	-78.000	-69.209	50.731
300	9.673	10.660	10.600	.018	-78.001	-69.155	50.378
400	10.679	13.598	10.993	1.042	-77.985	-66.205	36.172
500	11.233	16.045	11.767	2.139	-77.933	-63.269	27.654
600	11.609	18.128	12.658	3.282	-77.873	-60.338	21.978
700	11.902	19.940	13.571	4.458	-77.825	-57.424	17.928
800	12.150	21.546	14.470	5.661	-77.796	-54.506	14.890
900	12.371	22.990	15.338	6.887	-77.792	-51.597	12.529
999	12.575	24.291	16.161	8.122	-77.814	-48.717	10.658
999	12.575	24.291	16.161	8.122	-78.529	-48.717	10.658
1000	12.577	24.304	16.169	8.135	-78.529	-48.689	10.641
1071	12.715	25.172	16.737	9.033	-78.548	-46.565	9.502
1071	12.715	25.172	16.737	9.033	-79.853	-46.565	9.502
1100	12.772	25.512	16.964	9.403	-79.859	-45.663	9.072
1200	12.960	26.632	17.725	10.689	-79.874	-42.559	7.751
1300	13.143	27.676	18.450	11.994	-79.875	-39.450	6.632
1400	13.322	28.657	19.144	13.318	-79.863	-36.338	5.672
1500	13.498	29.582	19.809	14.659	-79.838	-33.232	4.842
1600	13.672	30.459	20.448	16.017	-79.799	-30.130	4.115
1700	13.845	31.293	21.062	17.393	-79.745	-27.020	3.474
1800	14.017	32.089	21.652	18.786	-79.677	-23.929	2.905
1900	14.187	32.851	22.222	20.196	-79.595	-20.828	2.396
2000	14.357	33.583	22.771	21.624	-79.496	-17.741	1.939

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 999 K, γ - δ transition point of Ce; ΔH° = 0.715 kcal/mol.
1071 K, melting point of Ce; ΔH° = 1.305 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.100 + 1.650\times10^{-3}T - 1.730\times10^{5}T^{-2}$
$H° - H°_{298} = 11.100\times10^{-3}T + 0.825\times10^{-6}T^{2} + 1.730\times10^{2}T^{-1} - 3.963$

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf° = -79.347 + 2.757\times10^{-3}T - 1.417\times10^{-6}T^{2} + 194.150T^{-1}$
$\Delta Gf° = -79.347 - 2.757\times10^{-3}T\ln T + 1.417\times10^{-6}T^{2} + 97.075T^{-1} + 48.194\times10^{-3}T$
999-1071 K: $\Delta Hf° = -78.087 - 1.148\times10^{-3}T + 0.530\times10^{-6}T^{2} + 176.950T^{-1}$
$\Delta Gf° = -78.087 + 1.148\times10^{-3}T\ln T - 0.530\times10^{-6}T^{2} + 88.475T^{-1} + 21.916\times10^{-3}T$
1071-2000 K: $\Delta Hf° = -79.370 - 1.168\times10^{-3}T + 0.530\times10^{-6}T^{2} + 176.950T^{-1}$
$\Delta Gf° = -79.370 + 1.168\times10^{-3}T\ln T - 0.530\times10^{-6}T^{2} + 88.475T^{-1} + 22.975\times10^{-3}T$

Source: Data from Barin (23) who estimated all except enthalpy of formation at 298 K.

$CeO(g)$
Cerium Monoxide (ideal gas)
[Formation: $Ce(c,l) + 0.5O_2(g) = CeO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	7.570	59.406	59.406	0	-32.000	-37.278	27.325
300	7.580	59.453	59.406	.014	-32.005	-37.311	27.181
400	7.920	61.680	59.708	.789	-32.244	-39.042	21.332
500	8.190	63.479	60.287	1.596	-32.496	-40.715	17.796
600	8.380	64.991	60.949	2.425	-32.771	-42.331	15.419
700	8.510	66.292	61.621	3.270	-33.079	-43.904	13.707
800	8.610	67.436	62.278	4.126	-33.425	-45.422	12.409
900	8.670	68.455	62.909	4.991	-33.811	-46.901	11.389
999	8.729	69.362	63.504	5.852	-34.232	-48.322	10.571
999	8.729	69.362	63.504	5.852	-34.947	-48.322	10.571
1000	8.730	69.371	63.510	5.861	-34.951	-48.337	10.564
1071	8.751	69.971	63.920	6.481	-35.266	-49.273	10.055
1071	8.751	69.971	63.920	6.481	-36.571	-49.273	10.055
1100	8.760	70.205	64.082	6.735	-36.701	-49.615	9.857
1200	8.800	70.969	64.624	7.614	-37.146	-50.772	9.247
1300	8.820	71.675	65.140	8.495	-37.595	-51.893	8.724
1400	8.840	72.329	65.630	9.378	-38.044	-52.972	8.269
1500	8.860	72.939	66.097	10.263	-38.496	-54.024	7.871
1600	8.870	73.512	66.543	11.150	-38.948	-55.048	7.519
1700	8.890	74.050	66.969	12.038	-39.402	-56.033	7.203
1800	8.900	74.559	67.377	12.928	-39.857	-57.007	6.922
1900	8.910	75.041	67.768	13.818	-40.315	-57.944	6.665
2000	8.920	75.498	68.144	14.709	-40.775	-58.864	6.432

Phase changes: 999 K, γ - δ transition point of Ce; ΔH° = 0.715 kcal/mol.
1071 K, melting point of Ce; ΔH° = 1.305 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.433 + 0.312 \times 10^{-3}T - 0.850 \times 10^{5}T^{-2}$
$H° - H°_{298} = 8.433 \times 10^{-3}T + 0.156 \times 10^{-6}T^{2} + 0.850 \times 10^{2}T^{-1} - 2.813$

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf° = -32.006 - 0.267 \times 10^{-3}T - 2.043 \times 10^{-6}T^{2} + 79.600T^{-1}$
$\Delta Gf° = -32.006 + 0.267 \times 10^{-3}T\ln T + 2.043 \times 10^{-6}T^{2} + 39.800T^{-1} - 20.262 \times 10^{-3}T$
999-1071 K: $\Delta Hf° = -30.746 - 4.172 \times 10^{-3}T - 0.095 \times 10^{-6}T^{2} + 62.400T^{-1}$
$\Delta Gf° = -30.746 + 4.172 \times 10^{-3}T\ln T + 0.095 \times 10^{-6}T^{2} + 31.200T^{-1} - 46.541 \times 10^{-3}T$
1071-2000 K: $\Delta Hf° = -32.029 - 4.192 \times 10^{-3}T - 0.095 \times 10^{-6}T^{2} + 62.400T^{-1}$
$\Delta Gf° = -32.029 + 4.192 \times 10^{-3}T\ln T + 0.095 \times 10^{-6}T^{2} + 31.200T^{-1} - 45.482 \times 10^{-3}T$

Source: Data from Pedley (396).

CoB(c,l)
Cobalt Boride
[Formation: $Co(c,l) + B(\beta) = CoB(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.800	7.600	7.600	0	-16.000	-15.705	11.512
300	8.846	7.655	7.602	.016	-16.000	-15.702	11.438
400	10.527	10.462	7.972	.996	-15.951	-15.616	8.532
500	11.423	12.915	8.721	2.097	-15.912	-15.530	6.788
600	12.054	15.056	9.603	3.272	-15.904	-15.458	5.630
700	12.594	16.955	10.519	4.505	-15.917	-15.383	4.803
700	12.594	16.955	10.519	4.505	-16.025	-15.383	4.803
800	13.115	18.671	11.432	5.791	-16.037	-15.286	4.176
900	13.651	20.246	12.325	7.129	-16.068	-15.191	3.689
1000	14.220	21.714	13.192	8.522	-16.117	-15.101	3.300
1100	14.833	23.097	14.030	9.974	-16.186	-14.995	2.979
1200	15.497	24.416	14.841	11.490	-16.280	-14.883	2.711
1300	16.215	25.685	15.627	13.075	-16.420	-14.763	2.482
1394	16.943	26.841	16.344	14.633	-16.636	-14.642	2.296
1400	16.989	26.914	16.389	14.735	-16.643	-14.633	2.284
1500	17.821	28.114	17.131	16.475	-16.556	-14.492	2.111
1600	18.713	29.293	17.855	18.301	-16.338	-14.375	1.963
1700	19.666	30.455	18.561	20.220	-16.019	-14.260	1.833
1748	20.145	31.010	18.896	21.175	-15.835	-14.221	1.778
1748	21.750	39.282	18.896	35.635	-1.375	-14.221	1.778
1768	21.750	39.530	19.128	36.069	-1.262	-14.357	1.775
1768	21.750	39.530	19.128	36.069	-4.962	-14.357	1.775
1800	21.750	39.919	19.493	36.766	-4.862	-14.524	1.763
1850	21.750	40.515	20.054	37.853	-4.708	-14.795	1.748

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.
1748 K, melting point of CoB; ΔH° = 14.460 kcal/mol.
1768 K, melting point of Co; ΔH° = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1748 K: $Cp^\circ = 8.538 + 6.194\times10^{-3}T - 1.409\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 8.538\times10^{-3}T + 3.097\times10^{-6}T^{2} + 1.409\times10^{2}T^{-1} - 3.293$
1748-1850 K: $Cp^\circ = 21.750$
$H^\circ - H^\circ_{298} = 21.750\times10^{-3}T - 2.384$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -15.393 - 1.186\times10^{-3}T + 0.628\times10^{-6}T^{2} - 92.200T^{-1}$
$\Delta Gf^\circ = -15.393 + 1.186\times10^{-3}T\ln T - 0.628\times10^{-6}T^{2} - 46.100T^{-1} - 7.097\times10^{-3}T$
700-1394 K: $\Delta Hf^\circ = -21.925 + 7.300\times10^{-3}T - 3.010\times10^{-6}T^{2} + 1494.200T^{-1}$
$\Delta Gf^\circ = -21.925 - 7.300\times10^{-3}T\ln T + 3.010\times10^{-6}T^{2} + 747.100T^{-1} + 53.661\times10^{-3}T$
1394-1748 K: $\Delta Hf^\circ = -9.447 - 10.610\times10^{-3}T + 3.998\times10^{-6}T^{2} - 80.600T^{-1}$
$\Delta Gf^\circ = -9.447 + 10.610\times10^{-3}T\ln T - 3.998\times10^{-6}T^{2} - 40.300T^{-1} - 74.783\times10^{-3}T$
1748-1768 K: $\Delta Hf^\circ = -8.538 + 2.602\times10^{-3}T + 0.901\times10^{-6}T^{2} - 221.500T^{-1}$
$\Delta Gf^\circ = -8.538 - 2.602\times10^{-3}T\ln T - 0.901\times10^{-6}T^{2} - 110.750T^{-1} + 17.950\times10^{-3}T$
1768-1850 K: $\Delta Hf^\circ = -12.402 + 5.511\times10^{-3}T - 0.692\times10^{-6}T^{2} - 221.500T^{-1}$
$\Delta Gf^\circ = -12.402 - 5.511\times10^{-3}T\ln T + 0.692\times10^{-6}T^{2} - 110.750T^{-1} + 39.071\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Sato (435). Other data based on Sidorenko (458).

$Co_2B(c)$
Dicobalt Boride
[Formation: $2Co(c) + B(\beta) = Co_2B(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.096	14.300	14.300	0	-11.300	-10.862	7.962
300	14.153	14.387	14.300	.026	-11.301	-10.856	7.909
400	16.345	18.793	14.885	1.563	-11.309	-10.718	5.856
500	17.646	22.590	16.056	3.267	-11.322	-10.557	4.614
600	18.597	25.895	17.427	5.081	-11.367	-10.404	3.790
700	19.382	28.822	18.851	6.980	-11.442	-10.242	3.198
700	19.382	28.822	18.851	6.980	-11.658	-10.242	3.198
800	20.079	31.456	20.264	8.954	-11.734	-10.027	2.739
900	20.725	33.859	21.642	10.995	-11.862	-9.809	2.382
1000	21.339	36.074	22.976	13.098	-12.055	-9.589	2.096
1100	21.932	38.136	24.261	15.262	-12.329	-9.322	1.852
1200	22.511	40.069	25.499	17.484	-12.708	-9.035	1.645
1300	23.080	41.894	26.691	19.764	-13.244	-8.712	1.465
1394	23.608	43.524	27.772	21.958	-13.990	-8.375	1.313
1400	23.642	43.625	27.839	22.100	-14.026	-8.349	1.303
1500	24.198	45.275	28.947	24.492	-14.277	-7.940	1.157

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 700 K, α – β transition point of Co; ΔH° = 0.108 kcal/mol.
1392 K, Curie temperature of Co; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 16.340 + 5.340\times10^{-3}T - 3.410\times10^{5}T^{-2}$
$H°-H°_{298} = 16.340\times10^{-3}T + 2.670\times10^{-6}T^{2} + 3.410\times10^{2}T^{-1} - 6.253$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -11.964 + 1.615\times10^{-3}T - 1.576\times10^{-6}T^{2} + 96.300T^{-1}$
$\Delta Gf° = -11.964 - 1.615\times10^{-3}T\ln T + 1.576\times10^{-6}T^{2} + 48.150T^{-1} + 11.889\times10^{-3}T$
700-1394 K: $\Delta Hf° = -25.028 + 18.587\times10^{-3}T - 8.852\times10^{-6}T^{2} + 3269.100T^{-1}$
$\Delta Gf° = -25.028 - 18.587\times10^{-3}T\ln T + 8.852\times10^{-6}T^{2} + 1634.550T^{-1} + 133.405\times10^{-3}T$
1394-1500 K: $\Delta Hf° = -0.072 - 17.233\times10^{-3}T + 5.164\times10^{-6}T^{2} + 119.500T^{-1}$
$\Delta Gf° = -0.072 + 17.233\times10^{-3}T\ln T - 5.164\times10^{-6}T^{2} + 59.750T^{-1} - 123.483\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Sato (435). Other data are those estimated by Barin (23).

$CoFe_2O_4(c)$
Cobalt Ferrite
[Formation: $Co(c) + 2Fe(c) + 2O_2(g) = CoFe_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	36.530	32.200	32.200	0	-272.400	-246.750	180.870
300	36.650	32.430	32.200	.070	-272.389	-246.588	179.637
400	41.800	43.880	33.730	4.060	-271.685	-238.094	130.087
500	44.700	53.530	36.770	8.380	-270.846	-229.797	100.443
600	47.100	61.900	40.267	12.980	-269.922	-221.666	80.741
700	49.000	69.310	43.896	17.790	-268.986	-213.698	66.719
700	49.000	69.310	43.896	17.790	-269.094	-213.698	66.719
784	55.600	75.010	46.923	22.020	-268.273	-207.095	57.730
800	51.800	76.090	47.227	23.090	-267.872	-205.634	56.176
900	46.400	81.790	50.757	27.930	-267.384	-197.886	48.053
1000	46.400	86.680	54.110	32.570	-267.524	-190.174	41.562

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
784 K, second order transition point of $CoFe_2O_4$; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 42.674 + 11.324x10^{-3}T - 8.462x10^{5}T^{-2}$
$H°-H°_{298} = 42.674x10^{-3}T + 5.662x10^{-6}T^{2} + 8.462x10^{2}T^{-1} - 16.065$
700-784 K: $Cp° = 13.973 + 49.036x10^{-3}T$
$H°-H°_{298} = 13.973x10^{-3}T + 24.518x10^{-6}T^{2} - 4.005$
784-1000 K: $Cp° = -1397.419 + 513.785x10^{-3}T + 3900.851x10^{5}T^{-2}$
$H°-H°_{298} = -1397.419x10^{-3}T + 531.785x10^{-6}T^{2} - 3900.851x10^{2}T^{-1} + 1288.289$

Formation equations (kcal/mol):

298.15-700 K: $ΔHf° = -282.658 + 23.655x10^{-3}T - 9.263x10^{-6}T^{2} + 1201.200T^{-1}$
$ΔGf° = -282.658 - 23.655x10^{-3}TlnT + 9.263x10^{-6}T^{2} + 600.600T^{-1} + 245.695x10^{-3}T$
700-784 K: $ΔHf° = -277.130 + 3.440x10^{-3}T + 5.955x10^{-6}T^{2} + 1941.400T^{-1}$
$ΔGf° = -277.130 - 3.440x10^{-3}TlnT - 5.955x10^{-6}T^{2} + 970.700T^{-1} + 115.264x10^{-3}T$
784-1000 K: $ΔHf° = 1015.164 - 1407.952x10^{-3}T + 513.222x10^{-6}T^{2} - 388143.700T^{-1}$
$ΔGf° = 1015.164 + 1407.952x10^{-3}TlnT - 513.222x10^{-6}T^{2} - 194071.850T^{-1} - 10224.147x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Low-temperature heat capacities and entropy at 298 K from King (262). High-temperature data from Reznitskii (421).

CoH(g)
Cobalt Hydride (ideal gas)
[Formation: Co(c) + $0.5H_2$(g) = CoH(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	6.980	52.390	52.390	0	107.500	98.673	-72.328
300	6.980	52.430	52.390	.013	107.495	98.620	-71.844
400	7.050	54.440	52.655	.714	107.235	95.697	-52.286
500	7.220	56.020	53.166	1.427	106.944	92.856	-40.587
600	7.410	57.360	53.763	2.158	106.633	90.062	-32.804
700	7.600	58.510	54.356	2.908	106.304	87.326	-27.264
700	7.600	58.510	54.356	2.908	106.196	87.326	-27.264
800	7.770	59.540	54.944	3.677	105.860	84.655	-23.126
900	7.930	60.470	55.512	4.462	105.489	82.019	-19.917
1000	8.050	61.300	56.038	5.262	105.076	79.437	-17.361

Phase change: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 6.118 + 2.004\times10^{-3}T + 0.235\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.118\times10^{-3}T + 1.002\times10^{-6}T^{2} - 0.235\times10^{2}T^{-1} - 1.834$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = 108.307 - 2.111\times10^{-3}T - 0.985\times10^{-6}T^{2} - 26.850T^{-1}$

$\Delta Gf^\circ = 108.307 + 2.111\times10^{-3}T\ln T + 0.985\times10^{-6}T^{2} - 13.425T^{-1} - 44.483\times10^{-3}T$

700-1000 K: $\Delta Hf^\circ = 101.775 + 6.375\times10^{-3}T - 4.622\times10^{-6}T^{2} + 1559.550T^{-1}$

$\Delta Gf^\circ = 101.775 - 6.375\times10^{-3}T\ln T + 4.622\times10^{-6}T^{2} + 779.775T^{-1} + 16.275\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kant (234). Other data from Kharitonov (253).

$Co_3N(c)$
Tricobalt Nitride
[Formation: $3Co(c) + 0.5N_2(g) = Co_3N(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	21.972	23.600	23.600	0	2.000	8.209	-6.017
300	22.000	23.736	23.600	.041	2.001	8.251	-6.011
400	23.500	30.270	24.480	2.316	2.086	10.306	-5.631
500	25.000	35.676	26.194	4.741	2.195	12.363	-5.404
600	26.500	40.366	28.173	7.316	2.337	14.383	-5.239

*All data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 17.500 + 15.000\times10^{-3}T$
$H°- H°_{298} = 17.500\times10^{-3}T + 7.500\times10^{-6}T^2 - 5.884$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = 2.164 - 0.761\times10^{-3}T + 1.874\times10^{-6}T^2 - 30.850T^{-1}$
$\Delta Gf° = 2.164 + 0.761\times10^{-3}T\ln T - 1.874\times10^{-6}T^2 - 15.425T^{-1} + 16.669\times10^{-3}T$

Source: Data are those estimated by Barin (23).

CoO(g)
Cobalt Monoxide (ideal gas)
[Formation: $Co(c,l) + 0.5O_2(g) = CoO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	7.550	55.778	55.778	0	70.000	62.816	-46.045
300	7.550	55.825	55.778	.014	69.996	62.772	-45.729
400	7.920	58.049	56.079	.788	69.801	60.388	-32.994
500	8.200	59.849	56.659	1.595	69.588	58.064	-25.379
600	8.390	61.362	57.320	2.425	69.349	55.780	-20.318
700	8.520	62.666	57.993	3.271	69.078	53.538	-16.715
700	8.520	62.666	57.993	3.271	68.970	53.538	-16.715
800	8.620	63.811	58.650	4.129	68.676	51.356	-14.030
900	8.690	64.830	59.281	4.994	68.335	49.209	-11.949
1000	8.740	65.748	59.883	5.865	67.938	47.095	-10.292
1100	8.780	66.583	60.455	6.741	67.478	45.040	-8.948
1200	8.810	67.349	60.998	7.621	66.943	43.021	-7.835
1300	8.840	68.056	61.514	8.504	66.306	41.048	-6.901
1394	8.859	68.673	61.976	9.336	65.566	39.241	-6.152
1400	8.860	68.711	62.005	9.389	65.524	39.128	-6.108
1500	8.880	69.321	62.471	10.275	64.986	37.259	-5.429
1600	8.890	69.897	62.920	11.164	64.506	35.422	-4.838
1700	8.910	70.437	63.346	12.054	64.047	33.617	-4.322
1768	8.917	70.786	63.625	12.661	63.738	32.402	-4.005
1768	8.917	70.786	63.625	12.661	60.038	32.402	-4.005
1800	8.920	70.946	63.754	12.946	59.812	31.905	-3.874
1900	8.930	71.428	64.145	13.838	59.106	30.373	-3.494
2000	8.940	71.887	64.521	14.732	58.399	28.879	-3.156
2100	8.950	72.323	64.882	15.627	57.689	27.422	-2.854
2200	8.960	72.740	65.230	16.522	56.978	25.997	-2.582
2300	8.970	73.138	65.565	17.418	56.264	24.602	-2.338
2400	8.970	73.520	65.889	18.315	55.549	23.242	-2.116
2500	8.980	73.887	66.202	19.213	54.832	21.910	-1.915

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.
1768 K, melting point of Co; ΔH° = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 8.478 + 0.278\times10^{-3}T - 0.898\times10^{5}T^{-2}$
$H° - H°_{298} = 8.478\times10^{-3}T + 0.139\times10^{-6}T^{2} + 0.898\times10^{2}T^{-1} - 2.841$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = 70.023 - 0.138\times10^{-3}T - 1.890\times10^{-6}T^{2} + 55.600T^{-1}$
$\Delta Gf° = 70.023 + 0.138\times10^{-3}T\ln T + 1.890\times10^{-6}T^{2} + 27.800T^{-1} - 25.834\times10^{-3}T$
700-1394 K: $\Delta Hf° = 63.491 + 8.348\times10^{-3}T - 5.528\times10^{-6}T^{2} + 1642.000T^{-1}$
$\Delta Gf° = 63.491 - 8.348\times10^{-3}T\ln T + 5.528\times10^{-6}T^{2} + 821.000T^{-1} + 34.925\times10^{-3}T$
1394-1768 K: $\Delta Hf° = 75.969 - 9.562\times10^{-3}T + 1.480\times10^{-6}T^{2} + 67.200T^{-1}$
$\Delta Gf° = 75.969 + 9.562\times10^{-3}T\ln T - 1.480\times10^{-6}T^{2} + 33.600T^{-1} - 93.519\times10^{-3}T$
1768-2000 K: $\Delta Hf° = 72.105 - 6.653\times10^{-3}T - 0.112\times10^{-6}T^{2} + 67.200T^{-1}$
$\Delta Gf° = 72.105 + 6.653\times10^{-3}T\ln T + 0.112\times10^{-6}T^{2} + 33.600T^{-1} - 72.398\times10^{-3}T$
2000-2500 K: $\Delta Hf° = 72.773 - 7.208\times10^{-3}T + 0.034\times10^{-6}T^{2} - 225.200T^{-1}$
$\Delta Gf° = 72.773 + 7.208\times10^{-3}T\ln T - 0.034\times10^{-6}T^{2} - 112.600T^{-1} - 76.620\times10^{-3}T$

Source: Data from Pedley (396).

$CoSO_4(c)$
Cobalt Sulfate
[Reaction: $Co(c) + 0.5S_2(g) + 2O_2(g) = CoSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	24.670	28.060	28.060	0	-227.655	-196.533	144.061
300*	24.773	28.213	28.060	.046	-227.653	-196.338	143.030
400	28.625	35.921	29.086	2.734	-227.398	-185.937	101.590
500	30.874	42.568	31.134	5.717	-226.946	-175.616	76.761
600	32.466	48.344	33.531	8.888	-226.400	-165.400	60.246
700	33.746	53.447	36.018	12.200	-225.803	-155.282	48.481
700	33.746	53.447	36.018	12.200	-225.911	-155.282	48.481
800	34.861	58.028	38.488	15.632	-225.262	-145.234	39.676
900	35.880	62.193	40.894	19.169	-224.593	-135.272	32.848
964	36.500	64.679	42.392	21.485	-224.156	-128.945	29.233
964	36.495	65.213	42.392	22.000	-223.641	-128.945	29.233
1000	36.837	66.557	43.237	23.320	-223.394	-125.413	27.409
1100	37.759	70.112	45.521	27.050	-222.706	-115.640	22.975
1200	38.653	73.436	47.710	30.871	-222.023	-105.938	19.294
1300	39.528	76.564	49.810	34.780	-221.372	-96.295	16.188
1394	40.336	79.352	51.709	38.534	-220.839	-87.278	13.683
1400	40.388	79.525	51.828	38.776	-220.798	-86.703	13.535

*Data above 298 K estimated.

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
964 K, α - β transition point of $CoSO_4$; ΔH° = 0.515 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-964 K: $Cp° = 29.208 + 8.280\times10^{-3}T - 6.228\times10^{5}T^{-2}$
$H°-H°_{298} = 29.208\times10^{-3}T + 4.140\times10^{-6}T^{2} + 6.228\times10^{2}T^{-1} - 11.165$
964-1400 K: $Cp° = 29.444 + 8.062\times10^{-3}T - 6.698\times10^{5}T^{-2}$
$H°-H°_{298} = 29.444\times10^{-3}T + 4.031\times10^{-6}T^{2} + 6.698\times10^{2}T^{-1} - 10.825$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta Hr° = -231.056 + 5.576\times10^{-3}T + 1.197\times10^{-6}T^{2} + 486.650T^{-1}$
$\Delta Gr° = -231.056 - 5.576\times10^{-3}T\ln T - 1.197\times10^{-6}T^{2} + 243.325T^{-1} + 145.176\times10^{-3}T$
700-964 K: $\Delta Hr° = -237.588 + 14.062\times10^{-3}T - 2.441\times10^{-6}T^{2} + 2073.050T^{-1}$
$\Delta Gr° = -237.588 - 14.062\times10^{-3}T\ln T + 2.441\times10^{-6}T^{2} + 1036.525T^{-1} + 205.935\times10^{-3}T$
964-1394 K: $\Delta Hr° = -237.248 + 14.297\times10^{-3}T - 2.550\times10^{-6}T^{2} + 2120.050T^{-1}$
$\Delta Gr° = -237.248 - 14.297\times10^{-3}T\ln T + 2.550\times10^{-6}T^{2} + 1060.025T^{-1} + 207.073\times10^{-3}T$
1394-1400 K: $\Delta Hr° = -224.770 - 3.613\times10^{-3}T + 4.458\times10^{-6}T^{2} + 545.250T^{-1}$
$\Delta Gr° = -224.770 + 3.613\times10^{-3}T\ln T - 4.458\times10^{-6}T^{2} + 272.625T^{-1} + 78.629\times10^{-3}T$

Source: Data from DeKock (112) who estimated all above 298 K.

$CoSO_4 \cdot H_2O(c)$
Cobalt Sulfate Monohydrate
[Reaction: $Co(c) + 0.5S_2(g) + 2.5O_2(g) + H_2(g) = CoSO_4 \cdot H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H^\circ_{298})/T$	$H° - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	34.004	42.000	42.000	0	-302.155	-258.580	189.542
300	34.170	42.211	42.001	.063	-302.155	-258.308	188.175
350	38.668	47.816	42.433	1.884	-302.061	-251.010	156.736
400	43.165	53.273	43.448	3.930	-301.771	-243.734	133.168
450	47.662	58.617	44.839	6.200	-301.284	-236.502	114.860
500	52.159	63.871	46.479	8.696	-300.599	-229.338	100.242
550	56.656	69.053	48.297	11.416	-299.719	-222.254	88.314

*Entropy at 298 K and data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 7.366 + 89.640\times10^{-3}T - 0.078\times10^{5}T^{-2}$
$H° - H^\circ_{298} = 7.366\times10^{-3}T + 44.820\times10^{-6}T^{2} + 0.078\times10^{2}T^{-1} - 6.207$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -297.514 - 26.338\times10^{-3}T + 41.207\times10^{-6}T^{2} - 134.450T^{-1}$
$\Delta Gr° = -297.514 + 26.338\times10^{-3}T\ln T - 41.207\times10^{-6}T^{2} - 67.225T^{-1} - 6.430\times10^{-3}T$

Source: Data from DeKock (112) who estimated entropy at 298 K and data above 298 K.

$CoSO_4 \cdot 6H_2O(c)$
Cobalt Sulfate Hexahydrate
[Reaction: $Co(c) + 0.5S_2(g) + 5O_2(g) + 6H_2(g) = CoSO_4 \cdot 6H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	84.340	87.863	87.863	0	-656.685	-543.735	398.563
300*	84.759	88.386	87.866	.156	-656.690	-543.033	395.594
337	92.978	98.715	88.489	3.446	-656.607	-529.016	343.071
350	95.794	102.287	88.936	4.673	-656.512	-524.100	327.259
400	106.274	115.769	91.451	9.727	-655.846	-505.224	276.038
450	116.200	128.865	94.885	15.291	-654.720	-486.455	236.252
500	125.572	141.598	98.924	21.337	-653.154	-467.839	204.490
550	134.389	153.984	103.368	27.839	-651.176	-449.401	178.573

*Data above 298 K estimated.

Phase change: 337 K, $CoSo_4 \cdot 6H_2O$ dissociated to $CoSo_4 \cdot H_2O$ and saturated solution.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 41.412 + 174.720x10^{-3}T - 8.147x10^{5}T^{-2}$

$H°- H°_{298} = 41.412x10^{-3}T + 87.360x10^{-6}T^{2} + 8.147x10^{2}T^{-1} - 22.845$

Reaction equations (kcal/mol):

298.15-550 K: $ΔHr° = -653.270 - 42.646x10^{-3}T + 80.394x10^{-6}T^{2} + 641.950T^{-1}$

$ΔGr° = -653.270 + 42.646x10^{-3}TlnT - 80.394x10^{-6}T^{2} + 320.975T^{-1} + 144.758x10^{-3}T$

Source: Data from DeKock (112) who estimated all above 298 K.

$CoSO_4 \cdot 7H_2O(c)$
Cobalt Sulfate Heptahydrate
[Reaction: $Co(c) + 0.5S_2(g) + 5.5O_2(g) + 7H_2(g) = CoSO_4 \cdot 7H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	93.483	97.048	97.048	0	-727.455	-600.633	440.270
300	93.924	97.628	97.051	.173	-727.463	-599.846	436.982
317.78	98.144	103.156	97.237	1.881	-727.477	-592.281	407.330
350	105.746	112.996	98.236	5.166	-727.331	-578.582	361.279
400	117.421	127.880	101.018	10.745	-726.667	-557.372	304.530
450	128.949	142.377	104.810	16.905	-725.475	-536.272	260.446
500	140.331	156.554	109.278	23.638	-723.755	-515.336	225.250
550	151.565	170.457	114.210	30.936	-721.518	-494.599	196.533

Phase change: 317.78 K, $CoSO_4 \cdot 7H_2O$ dissociates to $CoSO_4 \cdot 6H_2O$ and saturated solution.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp^\circ = 28.964 + 224.408 \times 10^{-3}T - 2.123 \times 10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 28.964 \times 10^{-3}T + 112.204 \times 10^{-6}T^{2} + 2.123 \times 10^{2}T^{-1} - 19.322$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr^\circ = -717.433 - 65.165 \times 10^{-3}T + 104.567 \times 10^{-6}T^{2} + 33.450T^{-1}$

$\Delta Gr^\circ = -717.433 + 65.165 \times 10^{-3}T\ln T - 104.567 \times 10^{-6}T^{2} + 16.725T^{-1} + 51.451 \times 10^{-3}T$

Source: Data from DeKock (112).

$Co_3Se_4(c)$
Tricobalt Tetraselenide
[Reaction: $3Co(c) + 2Se_2(g) = Co_3Se_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	42.693	61.236	61.236	0	-87.600	-64.731	47.448
300	42.749	61.495	61.238	.077	-87.592	-64.587	47.051
400	45.003	74.137	62.937	4.480	-87.021	-57.016	31.152
500	46.998	84.371	66.227	9.072	-86.410	-49.565	21.665
600	49.455	93.163	70.005	13.895	-85.685	-42.271	15.397
700	51.730	100.947	73.877	18.949	-84.835	-35.102	10.959
700	51.730	100.947	73.877	18.949	-85.159	-35.102	10.959
800	56.028	108.108	77.719	24.311	-84.069	-28.011	7.652
900	63.140	115.080	81.480	30.240	-82.548	-21.096	5.123
1000	89.824	122.542	85.204	37.338	-80.010	-14.422	3.152
1005	251.000	123.151	85.386	37.954	-79.627	-14.090	3.064
1050	68.194	126.294	87.081	41.174	-78.518	-11.163	2.323

*Entropy at 298 K estimated.

Phase changes: 700 K, α − β transition point of Co; ΔH° = 0.108 kcal/mol.
1005 K, second-order transition point of Co_3Se_4; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1005 K: $Cp° = 7.747 + 63.184 \times 10^{-3}T + 14.318 \times 10^{5}T^{-2}$
$H° - H°_{298} = 7.747 \times 10^{-3}T + 31.592 \times 10^{-6}T^2 - 14.318 \times 10^{2}T^{-1} - 0.316$
1005-1050 K: $Cp° = 531.578 - 448.400 \times 10^{-3}T$
$H° - H°_{298} = 531.578 \times 10^{-3}T - 224.200 \times 10^{-6}T^2 - 269.834$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta Hr° = -76.148 - 28.584 \times 10^{-3}T + 26.899 \times 10^{-6}T^2 - 1586.400T^{-1}$
$\Delta Gr° = -76.148 + 28.584 \times 10^{-3}T\ln T - 26.899 \times 10^{-6}T^2 - 793.200T^{-1} - 107.623 \times 10^{-3}T$
700-1005 K: $\Delta Hr° = -95.744 - 3.126 \times 10^{-3}T + 15.985 \times 10^{-6}T^2 + 3172.800T^{-1}$
$\Delta Gr° = -95.744 + 3.126 \times 10^{-3}T\ln T - 15.985 \times 10^{-6}T^2 + 1586.400T^{-1} + 74.652 \times 10^{-3}T$
1005-1050 K: $\Delta Hr° = -365.262 + 520.705 \times 10^{-3}T - 239.807 \times 10^{-6}T^2 + 4604.600T^{-1}$
$\Delta Gr° = -365.262 - 520.705 \times 10^{-3}T\ln T + 239.807 \times 10^{-6}T^2 + 2302.300T^{-1} + 3706.159 \times 10^{-3}T$

Sources: Enthalpy of formation based on Morozova (340). Other data from Gronvold (186) who estimated entropy at 298 K.

CoSi(c,l)
Cobalt Silicide
[Formation: Co(c,l) + Si(c,l) = CoSi(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	10.600	10.300	10.300	0	-24.000	-23.589	17.291
300	10.630	10.370	10.303	.020	-24.000	-23.586	17.182
400	11.780	13.610	10.735	1.150	-23.991	-23.455	12.815
500	12.320	16.300	11.580	2.360	-23.982	-23.312	10.190
600	12.660	18.580	12.563	3.610	-23.996	-23.180	8.443
700	12.920	20.550	13.564	4.890	-24.035	-23.043	7.194
700	12.920	20.550	13.564	4.890	-24.143	-23.043	7.194
800	13.180	22.290	14.553	6.190	-24.200	-22.880	6.250
900	13.450	23.860	15.504	7.520	-24.290	-22.715	5.516
1000	13.740	25.290	16.410	8.880	-24.412	-22.532	4.924
1100	14.070	26.620	17.284	10.270	-24.576	-22.343	4.439
1200	14.450	27.860	18.110	11.700	-24.781	-22.129	4.030
1300	14.860	29.030	18.907	13.160	-25.062	-21.903	3.682
1394	15.302	30.074	19.616	14.578	-25.427	-21.653	3.395
1400	15.330	30.140	19.661	14.670	-25.444	-21.636	3.377
1500	15.840	31.220	20.400	16.230	-25.537	-21.382	3.115
1600	16.390	32.260	21.110	17.840	-25.525	-21.109	2.883
1687	16.921	33.140	21.706	19.290	-25.452	-20.846	2.701
1687	16.921	33.140	21.706	19.290	-37.534	-20.846	2.701
1700	17.000	33.270	21.794	19.510	-37.510	-20.714	2.663
1738	17.250	33.650	22.049	20.160	-37.435	-20.348	2.559
1738	20.000	43.250	22.049	36.850	-20.745	-20.348	2.559
1768	20.000	43.592	22.410	37.450	-20.599	-20.336	2.514
1768	20.000	43.592	22.410	37.450	-24.299	-20.336	2.514
1800	20.000	43.950	22.789	38.090	-24.223	-20.261	2.460
1900	20.000	45.040	23.940	40.090	-23.984	-20.064	2.308
2000	20.000	46.060	25.015	42.090	-23.746	-19.858	2.170

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.
1738 K, melting point of CoSi; ΔH° = 16.690 kcal/mol.
1768 K, melting point of Co; ΔH° = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1738 K: $Cp^\circ = 10.968 + 3.202\times10^{-3}T - 1.174\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.968\times10^{-3}T + 1.601\times10^{-6}T^2 + 1.174\times10^{2}T^{-1} - 3.806$
1738-2000 K: $Cp^\circ = 20.000$
$H^\circ - H^\circ_{298} = 20.000\times10^{-3}T + 2.090$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -24.064 + 0.288\times10^{-3}T - 0.527\times10^{-6}T^2 + 7.300T^{-1}$
$\Delta Gf^\circ = -24.064 - 0.288\times10^{-3}T\ln T + 0.527\times10^{-6}T^2 + 3.650T^{-1} + 3.036\times10^{-3}T$
700-1394 K: $\Delta Hf^\circ = -30.595 + 8.774\times10^{-3}T - 4.165\times10^{-6}T^2 + 1593.700T^{-1}$
$\Delta Gf^\circ = -30.595 - 8.774\times10^{-3}T\ln T + 4.165\times10^{-6}T^2 + 796.850T^{-1} + 63.794\times10^{-3}T$
1394-1687 K: $\Delta Hf^\circ = -18.117 - 9.136\times10^{-3}T + 2.843\times10^{-6}T^2 + 18.900T^{-1}$
$\Delta Gf^\circ = -18.117 + 9.136\times10^{-3}T\ln T - 2.843\times10^{-6}T^2 + 9.450T^{-1} - 64.650\times10^{-3}T$
1687-1738 K: $\Delta Hf^\circ = -30.546 - 9.557\times10^{-3}T + 3.194\times10^{-6}T^2 + 117.400T^{-1}$
$\Delta Gf^\circ = -30.546 + 9.557\times10^{-3}T\ln T - 3.194\times10^{-6}T^2 + 58.700T^{-1} - 59.836\times10^{-3}T$
1738-1768 K: $\Delta Hf^\circ = -24.650 - 0.525\times10^{-3}T + 1.593\times10^{-6}T^2$
$\Delta Gf^\circ = -24.650 + 0.525\times10^{-3}T\ln T - 1.593\times10^{-6}T^2 + 1.392\times10^{-3}T$
1768-2000 K: $\Delta Hf^\circ = -28.514 + 2.384\times10^{-3}T$
$\Delta Gf^\circ = -28.514 - 2.384\times10^{-3}T\ln T + 22.513\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Other data based on Kalishevich (226).

$CoSi_2$(c,l)
Cobalt Disilicide

[Formation: Co(c,l) + 2Si(c,l) = $CoSi_2$(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.420	10.230	10.230	0	-24.600	-22.826	16.732
300	10.441	10.295	10.232	.019	-24.610	-22.815	16.620
400	11.281	13.426	10.651	1.110	-25.147	-22.145	12.100
500	11.831	16.005	11.471	2.267	-25.737	-21.319	9.319
600	12.269	18.202	12.415	3.472	-26.368	-20.381	7.424
700	12.655	20.123	13.382	4.719	-27.031	-19.335	6.037
700	12.655	20.123	13.382	4.719	-27.139	-19.335	6.037
800	13.013	21.836	14.334	6.002	-27.818	-18.167	4.963
900	13.355	23.389	15.255	7.321	-28.539	-16.919	4.108
1000	13.686	24.813	16.140	8.673	-29.297	-15.580	3.405
1100	14.011	26.133	16.989	10.058	-30.103	-14.178	2.817
1200	14.331	27.365	17.802	11.475	-30.965	-12.695	2.312
1300	14.649	28.525	18.583	12.924	-31.907	-11.140	1.873
1394	14.945	29.558	19.289	14.315	-32.917	-9.601	1.505
1400	14.964	29.622	19.333	14.405	-32.975	-9.500	1.483
1500	15.277	30.665	20.054	15.917	-33.779	-7.822	1.140
1600	15.589	31.661	20.749	17.460	-34.502	-6.072	.829
1600	18.500	41.630	20.749	33.410	-18.552	-6.072	.829
1687	18.500	42.610	21.852	35.019	-18.905	-5.344	.692
1687	18.500	42.610	21.852	35.019	-43.069	-5.344	.692
1700	18.500	42.752	22.011	35.260	-43.104	-5.044	.648
1768	18.500	43.477	22.822	36.518	-43.290	-3.519	.435
1768	18.500	43.477	22.822	36.518	-46.990	-3.519	.435
1800	18.500	43.809	23.192	37.110	-47.157	-2.729	.331

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.
1600 K, melting point of $CoSi_2$; ΔH° = 15.950 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.
1768 K, melting point of Co; ΔH° = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 10.743 + 3.054\times10^{-3}T - 1.095\times10^{5}T^{-2}$
$H°-H°_{298} = 10.743\times10^{-3}T + 1.527\times10^{-6}T^{2} + 1.095\times10^{2}T^{-1} - 3.706$
1600-1800 K: $Cp° = 18.500$
$H°-H°_{298} = 18.500\times10^{-3}T + 3.810$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -22.509 - 5.616\times10^{-3}T - 0.952\times10^{-6}T^{2} - 99.100T^{-1}$
$\Delta Gf° = -22.509 + 5.616\times10^{-3}T\ln T + 0.952\times10^{-6}T^{2} - 49.550T^{-1} - 32.789\times10^{-3}T$
700-1394 K: $\Delta Hf° = -29.040 + 2.870\times10^{-3}T - 4.590\times10^{-6}T^{2} + 1487.300T^{-1}$
$\Delta Gf° = -29.040 - 2.870\times10^{-3}T\ln T + 4.590\times10^{-6}T^{2} + 743.650T^{-1} + 27.970\times10^{-3}T$
1394-1600 K: $\Delta Hf° = -16.562 - 15.040\times10^{-3}T + 2.418\times10^{-6}T^{2} - 87.500T^{-1}$
$\Delta Gf° = -16.562 + 15.040\times10^{-3}T\ln T - 2.418\times10^{-6}T^{2} - 43.750T^{-1} - 100.475\times10^{-3}T$
1600-1687 K: $\Delta Hf° = -9.046 - 7.283\times10^{-3}T + 0.891\times10^{-6}T^{2} - 197.000T^{-1}$
$\Delta Gf° = -9.046 + 7.283\times10^{-3}T\ln T - 0.891\times10^{-6}T^{2} - 98.500T^{-1} - 50.365\times10^{-3}T$
1687-1768 K: $\Delta Hf° = -33.904 - 8.125\times10^{-3}T + 1.593\times10^{-6}T^{2}$
$\Delta Gf° = -33.904 + 8.125\times10^{-3}T\ln T - 1.593\times10^{-6}T^{2} - 40.737\times10^{-3}T$
1768-1800 K: $\Delta Hf° = -37.768 - 5.216\times10^{-3}T$
$\Delta Gf° = -37.768 + 5.216\times10^{-3}T\ln T - 19.615\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Low-temperature heat capacities and entropy at 298 K from Kalishevich (229). High-temperature data based on Kalishevich (230).

$Co_2SiO_4(c)$
Cobalt Silicate
[Formation: $2Co(c) + Si(c) + 2O_2(g) = Co_2SiO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	31.911	34.082	34.082	0	-337.400	-312.717	229.225
300	32.014	34.280	34.083	.059	-337.398	-312.562	227.698
400	36.263	44.126	35.396	3.492	-337.120	-304.330	166.276
500	38.904	52.522	38.002	7.260	-336.670	-296.170	129.454
600	40.695	59.783	41.041	11.245	-336.151	-288.120	104.946
700	41.961	66.157	44.184	15.381	-335.618	-280.163	87.470
700	41.961	66.157	44.184	15.381	-335.834	-280.163	87.470
800	42.865	71.823	47.292	19.625	-335.295	-272.241	74.372
900	43.496	76.910	50.304	23.945	-334.823	-264.391	64.202
1000	43.910	81.516	53.199	28.317	-334.441	-256.597	56.079

Phase change: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 38.970 + 6.214\times10^{-3}T - 7.922\times10^{5}T^{-2}$

$H°-H°_{298} = 38.970\times10^{-3}T + 3.107\times10^{-6}T^{2} + 7.922\times10^{2}T^{-1} - 14.552$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -341.818 + 8.829\times10^{-3}T - 1.804\times10^{-6}T^{2} + 580.100T^{-1}$

$\Delta Gf° = -341.818 - 8.829\times10^{-3}T\ln T + 1.804\times10^{-6}T^{2} + 290.050T^{-1} + 144.108\times10^{-3}T$

700-1000 K: $\Delta Hf° = -354.881 + 25.801\times10^{-3}T - 9.080\times10^{-6}T^{2} + 3752.900T^{-1}$

$\Delta Gf° = -354.881 - 25.801\times10^{-3}T\ln T + 9.080\times10^{-6}T^{2} + 1876.450T^{-1} + 265.625\times10^{-3}T$

Sources: Enthalpy of formation at 298 K, entropy at 298 K, and low-temperature heat capacities from Robie (427). High-temperature data based on Robie (426).

Co_3Te_4(c)
Tricobalt Tetratelluride
[Reaction: $3Co(c) + 2Te_2(g) = Co_3Te_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	42.749	72.107	72.107	0	-121.960	-100.143	73.406
300	42.833	72.373	72.116	.077	-121.948	-100.010	72.856
400	45.388	85.078	73.826	4.501	-121.124	-92.831	50.720
500	47.684	95.452	77.140	9.156	-120.226	-85.842	37.521
600	49.686	104.328	80.948	14.028	-119.256	-79.049	28.793
700	52.017	112.147	84.857	19.103	-118.223	-72.439	22.616
700	52.017	112.147	84.857	19.103	-118.547	-72.439	22.616
800	55.461	119.315	88.725	24.472	-117.326	-65.930	18.011
900	59.073	126.049	92.496	30.198	-115.922	-59.590	14.470
1000	65.583	132.573	96.187	36.386	-114.252	-53.455	11.682

*Entropy at 298 K estimated.

Phase change: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 31.146 + 30.770\times10^{-3}T + 2.159\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.146\times10^{-3}T + 15.385\times10^{-6}T^2 - 2.159\times10^{2}T^{-1} - 9.930$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta Hr^\circ = -121.431 - 1.055\times10^{-3}T + 8.868\times10^{-6}T^2 - 299.100T^{-1}$

$\Delta Gr^\circ = -121.431 + 1.055\times10^{-3}T\ln T - 8.868\times10^{-6}T^2 - 149.550T^{-1} + 69.713\times10^{-3}T$

700-1000 K: $\Delta Hr^\circ = -141.026 + 24.403\times10^{-3}T - 2.046\times10^{-6}T^2 + 4460.100T^{-1}$

$\Delta Gr^\circ = -141.026 - 24.403\times10^{-3}T\ln T + 2.046\times10^{-6}T^2 + 2230.050T^{-1} + 251.988\times10^{-3}T$

Sources: Enthalpy of formation from Morozova (341). Other data from Gronvold (186) who estimated entropy at 298 K.

$CoWO_4(c)$
Cobalt Tungstate
[Formation: $Co(c) + W(c) + 2O_2(g) = CoWO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	28.410	30.080	30.080	0	-270.000	-245.280	179.793
300	28.507	30.256	30.080	.053	-269.995	-245.124	178.571
400	32.091	39.012	31.250	3.105	-269.568	-236.897	129.433
500	33.989	46.395	33.561	6.417	-268.979	-228.791	100.003
600	35.222	52.708	36.240	9.881	-268.335	-220.817	80.432
700	36.141	58.209	38.993	13.451	-267.675	-212.948	66.485
700	36.141	58.209	38.993	13.451	-267.783	-212.948	66.485
800	36.893	63.086	41.706	17.104	-267.110	-205.163	56.047
900	37.548	67.469	44.328	20.827	-266.456	-197.454	47.948
985	38.056	70.881	46.475	24.040	-265.917	-190.972	42.372
985	40.000	71.328	46.475	24.480	-265.477	-190.972	42.372
1000	40.000	71.932	46.852	25.080	-265.356	-189.838	41.489
1100	40.000	75.744	49.308	29.080	-264.604	-182.306	36.220

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
985 K, α - β transition point of $CoWO_4$; ΔH° = 0.440 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-985 K: $Cp° = 34.365 + 4.424\times10^{-3}T - 6.468\times10^{5}T^{-2}$
$H° - H°_{298} = 34.365\times10^{-3}T + 2.212\times10^{-6}T^{2} + 6.468\times10^{2}T^{-1} - 12.612$
985-1100 K: $Cp° = 40.000$
$H° - H°_{298} = 40.000\times10^{-3}T - 14.920$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -274.383 + 9.089\times10^{-3}T - 0.942\times10^{-6}T^{2} + 523.800T^{-1}$
$\Delta Gf° = -274.383 - 9.089\times10^{-3}T\ln T + 0.942\times10^{-6}T^{2} + 261.900T^{-1} + 146.169\times10^{-3}T$
700-985 K: $\Delta Hf° = -280.915 + 17.575\times10^{-3}T - 4.580\times10^{-6}T^{2} + 2110.200T^{-1}$
$\Delta Gf° = -280.915 - 17.575\times10^{-3}T\ln T + 4.580\times10^{-6}T^{2} + 1055.100T^{-1} + 206.927\times10^{-3}T$
985-1100 K: $\Delta Hf° = -283.223 + 23.210\times10^{-3}T - 6.792\times10^{-6}T^{2} + 1463.400T^{-1}$
$\Delta Gf° = -283.223 - 23.210\times10^{-3}T\ln T + 6.792\times10^{-6}T^{2} + 731.700T^{-1} + 246.265\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Rezukhina (423). Low-temperature heat capacities and entropy at 298 K from Landee (293). High-temperature data based on Yakovleva (536).

CrB(c)
Chromium Boride
[Formation: Cr(c) + B(β) = CrB(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.561	5.750	5.750	0	-18.000	-17.609	12.908
300	8.601	5.803	5.750	.016	-17.999	-17.607	12.826
311.5	8.780	6.130	5.758	.116	-17.997	-17.592	12.342
400	10.158	8.515	6.110	.962	-17.951	-17.485	9.553
500	11.082	10.888	6.834	2.027	-17.915	-17.369	7.592
600	11.758	12.970	7.687	3.170	-17.905	-17.263	6.288
700	12.316	14.826	8.576	4.375	-17.905	-17.153	5.355
800	12.812	16.503	9.463	5.632	-17.906	-17.044	4.656
900	13.271	18.039	10.332	6.936	-17.901	-16.937	4.113
1000	13.708	19.460	11.175	8.285	-17.892	-16.832	3.679
1100	14.130	20.786	11.989	9.677	-17.890	-16.731	3.324
1200	14.542	22.034	12.775	11.111	-17.899	-16.620	3.027

*Enthalpy of formation and entropy at 298 K estimated.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 10.150 + 3.800\text{x}10^{-3}T - 2.420\text{x}10^{5}T^{-2}$
$H° - H°_{298} = 10.150\text{x}10^{-3}T + 1.900\text{x}10^{-6}T^{2} + 2.420\text{x}10^{2}T^{-1} - 4.007$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -19.381 + 8.235\text{x}10^{-3}T - 12.859\text{x}10^{-6}T^{2} + 20.500T^{-1}$
$\Delta Gf° = -19.381 - 8.235\text{x}10^{-3}T\ln T + 12.859\text{x}10^{-6}T^{2} + 10.250T^{-1} + 48.912\text{x}10^{-3}T$
311.5-1200 K: $\Delta Hf° = -18.383 + 1.068\text{x}10^{-3}T - 0.583\text{x}10^{-6}T^{2} + 34.100T^{-1}$
$\Delta Gf° = -18.383 - 1.068\text{x}10^{-3}T\ln T + 0.583\text{x}10^{-6}T^{2} + 17.050T^{-1} + 8.315\text{x}10^{-3}T$

Source: Data from Barin (23) who estimated enthalpy of formation and entropy at 298 K.

$CrB_2(c)$
Chromium Diboride
[Formation: $Cr(c) + 2B(\beta) = CrB_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	12.809	6.250	6.250	0	-28.500	-27.838	20.406
300	12.829	6.329	6.252	.023	-28.497	-27.834	20.277
311.5	12.952	6.814	6.264	.171	-28.478	-27.808	19.510
400	13.901	10.167	6.767	1.360	-28.375	-27.638	15.100
500	14.973	13.384	7.776	2.804	-28.367	-27.449	11.998
600	16.045	16.209	8.952	4.354	-28.425	-27.266	9.932
700	17.117	18.762	10.172	6.013	-28.489	-27.062	8.449
800	18.189	21.118	11.396	7.778	-28.528	-26.854	7.336
900	19.261	23.322	12.600	9.650	-28.524	-26.645	6.470
1000	20.333	25.407	13.777	11.630	-28.472	-26.439	5.778
1100	21.405	27.395	14.925	13.717	-28.379	-26.251	5.215
1200	22.477	29.304	16.045	15.911	-28.247	-26.056	4.745

*Entropy at 298 K estimated.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K:

$$Cp^\circ = 9.613 + 10.720\times10^{-3}T$$

$$H^\circ - H^\circ_{298} = 9.613\times10^{-3}T + 5.360\times10^{-6}T^2 - 3.343$$

Formation equations (kcal/mol):

298.15-311.5 K:

$$\Delta Hf^\circ = -27.004 + 2.975\times10^{-3}T - 10.091\times10^{-6}T^2 - 443.000T^{-1}$$

$$\Delta Gf^\circ = -27.004 - 2.975\times10^{-3}T\ln T + 10.091\times10^{-6}T^2 - 221.500T^{-1} + 13.636\times10^{-3}T$$

311.5-1200 K:

$$\Delta Hf^\circ = -26.006 - 4.192\times10^{-3}T + 2.185\times10^{-6}T^2 - 429.400T^{-1}$$

$$\Delta Gf^\circ = -26.006 + 4.192\times10^{-3}T\ln T - 2.185\times10^{-6}T^2 - 214.700T^{-1} - 26.961\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Topor (499). Other data from Barin (23) who estimated entropy at 298 K.

$Cr_3C_2(c)$
Trichromium Dicarbide
[Formation: $3Cr(c) + 2C(c) = Cr_3C_2(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	23.530	20.420	20.420	0	-22.500	-22.716	16.651
300	23.625	20.566	20.420	.044	-22.494	-22.721	16.552
311.5	24.051	21.463	20.441	.318	-22.469	-22.729	15.947
400	27.328	27.940	21.403	2.615	-22.154	-22.844	12.481
500	29.412	34.278	23.358	5.460	-21.809	-23.051	10.075
600	30.886	39.777	25.647	8.478	-21.519	-23.324	8.496
700	32.072	44.630	28.019	11.628	-21.278	-23.643	7.381
800	33.104	48.981	30.372	14.887	-21.073	-23.995	6.555
900	34.047	52.935	32.663	18.245	-20.879	-24.374	5.919
1000	34.935	56.569	34.874	21.695	-20.699	-24.778	5.415
1100	35.787	59.939	37.002	25.231	-20.569	-25.168	5.000
1200	36.614	63.088	39.046	28.851	-20.497	-25.599	4.662
1300	37.423	66.051	41.010	32.553	-20.508	-26.052	4.380
1400	38.220	68.853	42.899	36.336	-20.570	-26.491	4.135
1500	39.008	71.517	44.719	40.197	-20.683	-26.876	3.916
1600	39.788	74.060	46.474	44.137	-20.867	-27.283	3.727
1700	40.563	76.495	48.169	48.155	-21.115	-27.713	3.563
1800	41.334	78.835	49.807	52.250	-21.416	-28.056	3.406
1900	42.102	81.091	51.396	56.421	-21.774	-28.434	3.271
2000	42.866	83.270	52.935	60.670	-22.159	-28.759	3.143

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 28.043 + 7.486\times10^{-3}T - 5.935\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 28.043\times10^{-3}T + 3.743\times10^{-6}T^{2} + 5.935\times10^{2}T^{-1} - 10.684$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -28.555 + 29.431\times10^{-3}T - 39.990\times10^{-6}T^{2} + 248.900T^{-1}$

$\Delta Gf^\circ = -28.555 - 29.431\times10^{-3}T\ln T + 39.990\times10^{-6}T^{2} + 124.450T^{-1} + 173.945\times10^{-3}T$

311.5-2000 K: $\Delta Hf^\circ = -25.562 + 7.930\times10^{-3}T - 3.162\times10^{-6}T^{2} + 289.700T^{-1}$

$\Delta Gf^\circ = -25.562 - 7.930\times10^{-3}T\ln T + 3.162\times10^{-6}T^{2} + 144.850T^{-1} + 52.152\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mah (318). Low-temperature heat capacities and entropy at 298 K from Kelley (245). High-temperature data based on Kelley (245) and Oriani (374).

Cr_7C_3(c)
Heptachromium Tricarbide
[Formation: $7Cr(c) + 3C(c) = Cr_7C_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	50.052	48.000	48.000	0	-43.300	-44.592	32.687
300	50.207	48.310	48.000	.093	-43.289	-44.608	32.496
311.5	50.906	50.212	48.047	.674	-43.249	-44.657	31.331
400	56.284	63.675	50.055	5.448	-42.733	-45.123	24.654
500	60.009	76.660	54.112	11.274	-42.212	-45.772	20.006
600	62.766	87.855	58.825	17.418	-41.805	-46.517	16.944
700	65.039	97.705	63.688	23.812	-41.492	-47.321	14.774
800	67.038	106.523	68.502	30.417	-41.248	-48.173	13.160
900	68.869	114.526	73.177	37.214	-41.022	-49.053	11.911
1000	70.595	121.872	77.684	44.188	-40.833	-49.970	10.921
1100	72.260	128.679	82.014	51.331	-40.764	-50.848	10.102
1200	73.893	135.037	86.171	58.639	-40.838	-51.768	9.428
1300	75.519	141.015	90.162	66.109	-41.115	-52.732	8.865
1400	77.159	146.672	93.998	73.743	-41.521	-53.646	8.374
1500	78.831	152.052	97.691	81.542	-42.048	-54.415	7.928
1600	80.553	157.194	101.250	89.511	-42.745	-55.215	7.542
1700	82.340	162.131	104.687	97.655	-43.585	-56.055	7.206
1800	84.209	166.890	108.012	105.981	-44.538	-56.681	6.882
1900	86.174	171.495	111.232	114.500	-45.600	-57.363	6.598
2000	88.251	175.967	114.357	123.220	-46.696	-57.920	6.329

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 55.859 + 15.710\times10^{-3}T - 9.326\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 55.859\times10^{-3}T + 7.855\times10^{-6}T^{2} + 9.326\times10^{2}T^{-1} - 20.481$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -55.803 + 64.961\times10^{-3}T - 92.912\times10^{-6}T^{2} + 415.700T^{-1}$

$\Delta Gf^\circ = -55.803 - 64.961\times10^{-3}T\ln T + 92.912\times10^{-6}T^{2} + 207.850T^{-1} + 377.683\times10^{-3}T$

311.5-2000 K: $\Delta Hf^\circ = -48.819 + 14.792\times10^{-3}T - 6.980\times10^{-6}T^{2} + 510.900T^{-1}$

$\Delta Gf^\circ = -48.819 - 14.792\times10^{-3}T\ln T + 6.980\times10^{-6}T^{2} + 255.450T^{-1} + 93.500\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mah (318). Other data based on Kelley (245).

$Cr_{23}C_6(c)$
Chromium Carbide
[Formation: $23Cr(c) + 6C(c) = Cr_{23}C_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	149.200	145.800	145.800	0	-94.700	-96.971	71.081
300	149.609	146.724	145.804	.276	-94.678	-97.010	70.671
311.5	151.683	152.391	145.943	2.008	-94.631	-97.094	68.121
400	167.644	192.513	151.928	16.234	-93.547	-97.933	53.507
500	179.187	231.242	164.018	33.612	-92.377	-99.127	43.328
600	187.400	264.675	178.072	51.962	-91.423	-100.550	36.625
700	193.723	294.055	192.585	71.029	-90.701	-102.110	31.880
800	199.065	320.279	206.936	90.674	-90.186	-103.782	28.352
900	204.010	344.013	220.869	110.830	-89.742	-105.507	25.620
1000	208.904	365.760	234.285	131.475	-89.435	-107.325	23.456
1100	213.919	385.905	247.164	152.615	-89.517	-109.021	21.660
1200	219.099	404.739	259.519	174.264	-90.048	-110.749	20.170
1300	224.406	422.486	271.379	196.439	-91.206	-112.640	18.936
1400	229.757	439.312	282.778	219.147	-92.759	-114.347	17.850
1500	235.065	455.345	293.752	242.389	-94.683	-115.564	16.838
1600	240.278	470.682	304.334	266.157	-97.175	-116.874	15.964
1700	245.419	485.404	314.556	290.442	-100.164	-118.289	15.207
1800	250.623	499.578	324.444	315.242	-103.588	-118.996	14.448
1900	256.176	513.275	334.023	340.578	-107.449	-119.869	13.788
2000	262.554	526.572	343.320	366.505	-111.468	-120.312	13.147

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 166.747 + 46.076\times10^{-3}T - 27.810\times10^{5}T^{-2}$
$H°-H°_{298} = 166.747\times10^{-3}T + 23.038\times10^{-6}T^{2} + 27.810\times10^{2}T^{-1} - 61.091$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -136.117 + 210.223\times10^{-3}T - 305.099\times10^{-6}T^{2} + 1747.200T^{-1}$
$\Delta Gf° = -136.117 - 210.223\times10^{-3}T\ln T + 305.099\times10^{-6}T^{2} + 873.600T^{-1} + 1228.268\times10^{-3}T$
311.5-2000 K: $\Delta Hf° = -113.170 + 45.382\times10^{-3}T - 22.751\times10^{-6}T^{2} + 2060\ T^{-1}$
$\Delta Gf° = -113.170 - 45.382\times10^{-3}T\ln T + 22.751\times10^{-6}T^{2} + 1030\ T^{-1} + 294.523\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mah (318). Other data based on Kelley (245).

$Cr(CO)_6(g)$
Chromium Hexacarbonyl (ideal gas)
[Formation: $Cr(c) + 6C(c) + 3O_2(g) = Cr(CO)_6(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	48.804	114.875	114.875	0	-217.100	-203.379	149.079
300	48.925	115.177	114.875	.091	-217.082	-203.294	148.098
311.5	49.574	117.030	114.919	.657	-216.970	-202.767	142.261
350	51.746	122.940	115.483	2.610	-216.642	-201.031	125.528
400	53.939	129.998	116.861	5.255	-216.093	-198.845	108.642
450	55.730	136.457	118.684	7.998	-215.647	-196.716	95.537
500	57.254	142.409	120.763	10.823	-215.242	-194.634	85.073
550	58.592	147.930	122.985	13.720	-214.888	-192.587	76.526
600	59.788	153.080	125.280	16.680	-214.570	-190.573	69.415

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 50.819 + 18.082 \times 10^{-3}T - 6.584 \times 10^{5}T^{-2}$
$H°- H°_{298} = 50.819 \times 10^{-3}T + 9.041 \times 10^{-6}T^{2} + 6.584 \times 10^{2}T^{-1} - 18.164$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -217.625 + 10.829 \times 10^{-3}T - 11.131 \times 10^{-6}T^{2} - 511.000T^{-1}$
$\Delta Gf° = -217.625 - 10.829 \times 10^{-3}T\ln T + 11.131 \times 10^{-6}T^{2} - 255.500T^{-1} + 109.039 \times 10^{-3}T$
311.5-600 K: $\Delta Hf° = -216.628 + 3.662 \times 10^{-3}T + 1.145 \times 10^{-6}T^{2} - 497.400T^{-1}$
$\Delta Gf° = -216.628 - 3.662 \times 10^{-3}T\ln T - 1.145 \times 10^{-6}T^{2} - 248.700T^{-1} + 68.441 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Pittam (403). Other data from Pilcher (401).

CrGe(c)
Chromium Germanide
[Formation: Cr(c) + Ge(c,l) = CrGe(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	12.026	14.600	14.600	0	-2.450	-2.903	2.128
300	12.044	14.674	14.601	.022	-2.448	-2.908	2.119
311.5	12.134	15.129	14.612	.161	-2.440	-2.926	2.053
400	12.823	18.258	15.083	1.270	-2.356	-3.075	1.680
500	13.347	21.178	16.020	2.579	-2.259	-3.263	1.426
600	13.778	23.650	17.090	3.936	-2.160	-3.468	1.263
700	14.165	25.804	18.185	5.333	-2.057	-3.698	1.154
800	14.529	27.719	19.259	6.768	-1.948	-3.939	1.076
900	14.879	29.451	20.297	8.239	-1.833	-4.192	1.018
1000	15.221	31.036	21.292	9.744	-1.722	-4.468	.976
1100	15.557	32.503	22.246	11.283	-1.628	-4.744	.943
1200	15.889	33.871	23.158	12.855	-1.556	-5.025	.915
1210.4	15.923	34.008	23.251	13.020	-1.550	-5.051	.912
1210.4	15.923	34.008	23.251	13.020	-10.380	-5.051	.912
1300	16.219	35.156	24.032	14.461	-10.312	-4.665	.784

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp° = 12.107 + 3.204\times10^{-3}T - 0.906\times10^{5}T^{-2}$

$H°-H°_{298} = 12.107\times10^{-3}T + 1.602\times10^{-6}T^{2} + 0.906\times10^{2}T^{-1} - 4.056$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -4.304 + 9.334\times10^{-3}T - 12.931\times10^{-6}T^{2} + 65.700T^{-1}$

$\Delta Gf° = -4.304 - 9.334\times10^{-3}T\ln T + 12.931\times10^{-6}T^{2} + 32.850T^{-1} + 53.654\times10^{-3}T$

311.5-1210.4 K: $\Delta Hf° = -3.306 + 2.167\times10^{-3}T - 0.655\times10^{-6}T^{2} + 79.300T^{-1}$

$\Delta Gf° = -3.306 - 2.167\times10^{-3}T\ln T + 0.655\times10^{-6}T^{2} + 39.650T^{-1} + 13.057\times10^{-3}T$

1210.4-1300 K: $\Delta Hf° = -11.606 + 1.148\times10^{-3}T - 0.189\times10^{-6}T^{2} + 104.200T^{-1}$

$\Delta Gf° = -11.606 - 1.148\times10^{-3}T\ln T + 0.189\times10^{-6}T^{2} + 52.100T^{-1} + 13.236\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Eremenko (139). Low-temperature heat capacities and entropy at 298 K from Kalishevich (232). High-temperature data based on Shchipanova (444).

$Cr_{11}Ge_{19}$(c)
Chromium Germanide

[Formation: 11Cr(c) + 19Ge(c) = $Cr_{11}Ge_{19}$(c)]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	180.400	227.300	227.300	0	-52.200	-59.350	43.504
300	180.600	228.420	227.320	.330	-52.170	-59.430	43.294
311.5	181.428	235.229	227.487	2.412	-52.048	-59.708	41.891
400	187.800	281.420	234.470	18.780	-51.036	-62.028	33.890
500	193.500	323.960	248.260	37.850	-50.018	-64.843	28.342
600	198.600	359.690	263.923	57.460	-49.046	-67.814	24.701
700	203.400	390.670	279.870	77.560	-48.036	-71.087	22.194
800	208.000	418.130	295.467	98.130	-46.964	-74.452	20.339
900	212.600	442.900	310.500	119.160	-45.858	-77.907	18.918
1000	217.100	465.530	324.890	140.640	-44.848	-81.668	17.848
1100	221.500	486.430	338.639	162.570	-44.085	-85.335	16.954
1200	226.000	505.890	351.765	184.950	-43.613	-89.009	16.211

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 174.226 + 43.420\times10^{-3}T - 6.019\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 174.226\times10^{-3}T + 21.710\times10^{-6}T^{2} + 6.019\times10^{2}T^{-1} - 55.894$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -69.559 + 99.075\times10^{-3}T - 141.881\times10^{-6}T^{2} + 128.800T^{-1}$

$\Delta Gf^\circ = -69.559 - 99.075\times10^{-3}T\ln T + 141.881\times10^{-6}T^{2} + 64.400T^{-1} + 555.705\times10^{-3}T$

311.5-1200 K: $\Delta Hf^\circ = -58.584 + 20.238\times10^{-3}T - 6.845\times10^{-6}T^{2} + 278.400T^{-1}$

$\Delta Gf^\circ = -58.584 - 20.238\times10^{-3}T\ln T + 6.845\times10^{-6}T^{2} + 139.200T^{-1} + 109.132\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Eremenko (139). Low-temperature heat capacities and entropy at 298 K from Kalishevich (232). High-temperature data based on Shchipanova (444).

$CrN(c)$
Chromium Nitride
[Formation: $Cr(c,l) + 0.5N_2(g) = CrN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.590	9.013	9.013	0	-28.000	-22.180	16.258
300	12.283	9.090	9.013	.023	-27.993	-22.145	16.132
311.5	12.219	9.551	9.025	.164	-27.960	-21.921	15.379
400	11.730	12.376	9.464	1.165	-27.781	-20.228	11.052
500	11.890	15.010	10.318	2.346	-27.573	-18.362	8.026
600	12.050	17.192	11.287	3.543	-27.391	-16.537	6.023
700	12.210	19.062	12.268	4.756	-27.229	-14.740	4.602
800	12.360	20.702	13.222	5.984	-27.084	-12.966	3.542
900*	12.520	22.167	14.136	7.228	-26.949	-11.209	2.722
1000	12.680	23.495	15.007	8.488	-26.829	-9.470	2.070
1100	12.840	24.711	15.835	9.764	-26.733	-7.738	1.537
1200	13.000	25.835	16.622	11.056	-26.665	-6.010	1.095
1300	13.150	26.881	17.370	12.364	-26.633	-4.298	.722
1400	13.310	27.862	18.086	13.687	-26.630	-2.586	.404
1500	13.475	28.786	18.769	15.026	-26.652	-.857	.125
1600	13.630	29.660	19.422	16.381	-26.707	.865	-.118
1700	13.790	30.491	20.049	17.752	-26.791	2.579	-.332
1800	13.950	31.284	20.651	19.139	-26.902	4.321	-.525
1900	14.120	32.043	21.231	20.542	-27.041	6.053	-.696
2000	14.300	32.772	21.790	21.964	-27.194	7.804	-.853
2100	14.430	33.473	22.330	23.400	-27.372	9.562	-.995
2130	14.475	33.678	22.489	23.834	-27.429	10.089	-1.035
2130	14.475	33.678	22.489	23.834	-31.476	10.089	-1.035
2200	14.580	34.147	22.852	24.850	-31.420	11.447	-1.137
2300	14.750	34.799	23.357	26.317	-31.327	13.399	-1.273
2400	14.930	35.431	23.847	27.801	-31.218	15.340	-1.397
2500	15.075	36.043	24.322	29.302	-31.094	17.294	-1.512

*Data extrapolated above 800 K.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
2130 K, melting point of Cr; ΔH° = 4.047 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp^\circ = 10.064 + 2.216\times10^{-3}T + 1.658\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.064\times10^{-3}T + 1.108\times10^{-6}T^2 - 1.658\times10^{2}T^{-1} - 2.543$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -29.145 + 9.614\times10^{-3}T - 13.253\times10^{-6}T^2 - 161.850T^{-1}$
$\Delta Gf^\circ = -29.145 - 9.614\times10^{-3}T\ln T + 13.253\times10^{-6}T^2 - 80.925T^{-1} + 75.096\times10^{-3}T$
311.5-2000 K: $\Delta Hf^\circ = -28.148 + 2.446\times10^{-3}T - 0.977\times10^{-6}T^2 - 148.250T^{-1}$
$\Delta Gf^\circ = -28.148 - 2.446\times10^{-3}T\ln T + 0.977\times10^{-6}T^2 - 74.125T^{-1} + 34.498\times10^{-3}T$
2000-2130 K: $\Delta Hf^\circ = -26.811 + 1.382\times10^{-3}T - 0.711\times10^{-6}T^2 - 698.200T^{-1}$
$\Delta Gf^\circ = -26.811 - 1.382\times10^{-3}T\ln T + 0.711\times10^{-6}T^2 - 349.100T^{-1} + 26.344\times10^{-3}T$
2130-2500 K: $\Delta Hf^\circ = -28.239 - 3.659\times10^{-3}T + 1.080\times10^{-6}T^2 - 711.800T^{-1}$
$\Delta Gf^\circ = -28.239 + 3.659\times10^{-3}T\ln T - 1.080\times10^{-6}T^2 - 355.900T^{-1} - 7.802\times10^{-3}T$

Source: Data from Chase (83) who extrapolated data above 800 K.

CrN(g)
Chromium Nitride (ideal gas)
[Formation: Cr(c,l) + $0.5N_2(g)$ = CrN(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	7.350	55.076	55.076	0	120.700	112.787	-82.674
300	7.357	55.122	55.076	.014	120.697	112.737	-82.128
311.5	7.399	55.400	55.082	.099	120.675	112.432	-78.882
400	7.726	57.290	55.370	.768	120.522	110.110	-60.160
500	8.027	59.048	55.936	1.556	120.336	107.529	-47.000
600	8.250	60.532	56.580	2.371	120.137	104.987	-38.241
700	8.412	61.817	57.240	3.204	119.920	102.480	-31.995
800	8.532	62.948	57.883	4.052	119.684	100.005	-27.320
900	8.622	63.958	58.502	4.910	119.433	97.561	-23.691
1000	8.692	64.871	59.095	5.776	119.159	95.142	-20.793
1100	8.747	65.702	59.658	6.648	118.851	92.756	-18.429
1200	8.792	66.465	60.194	7.525	118.504	90.403	-16.464
1300	8.829	67.170	60.704	8.406	118.109	88.069	-14.806
1400	8.859	67.826	61.190	9.290	117.673	85.768	-13.389
1500	8.886	68.438	61.653	10.178	117.200	83.517	-12.168
1600	8.909	69.012	62.095	11.067	116.679	81.287	-11.103
1700	8.930	69.553	62.518	11.959	116.116	79.081	-10.166
1800	8.950	70.064	62.923	12.853	115.512	76.931	-9.341
1900	8.968	70.548	63.312	13.749	114.866	74.800	-8.604
2000	8.987	71.009	63.686	14.647	114.189	72.712	-7.946
2100	9.005	71.448	64.045	15.547	113.475	70.662	-7.354
2130	9.011	71.576	64.150	15.817	113.255	70.050	-7.187
2130	9.011	71.576	64.150	15.817	109.208	70.050	-7.187
2200	9.025	71.867	64.391	16.448	108.878	68.761	-6.831
2300	9.045	72.269	64.725	17.352	108.408	66.953	-6.362
2400	9.067	72.654	65.047	18.257	107.938	65.161	-5.934
2500	9.091	73.025	65.359	19.165	107.469	63.402	-5.543

*Data except enthalpy of formation at 298 K estimated.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
2130 K, melting point of Cr; ΔH° = 4.047 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp^\circ = 8.315 + 0.384\mathrm{x}10^{-3}T - 0.959\mathrm{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.315\mathrm{x}10^{-3}T + 0.192\mathrm{x}10^{-6}T^2 + 0.959\mathrm{x}10^{2}T^{-1} - 2.818$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = 119.280 + 7.865\mathrm{x}10^{-3}T - 14.170\mathrm{x}10^{-6}T^2 + 99.850T^{-1}$

$\Delta Gf^\circ = 119.280 - 7.865\mathrm{x}10^{-3}T\ln T + 14.170\mathrm{x}10^{-6}T^2 + 49.925T^{-1} + 18.245\mathrm{x}10^{-3}T$

311.5-2000 K: $\Delta Hf^\circ = 120.278 + 0.697\mathrm{x}10^{-3}T - 1.893\mathrm{x}10^{-6}T^2 + 113.450T^{-1}$

$\Delta Gf^\circ = 120.278 - 0.697\mathrm{x}10^{-3}T\ln T + 1.893\mathrm{x}10^{-6}T^2 + 56.725T^{-1} - 22.353\mathrm{x}10^{-3}T$

2000-2130 K: $\Delta Hf^\circ = 121.615 - 0.367\mathrm{x}10^{-3}T - 1.627\mathrm{x}10^{-6}T^2 - 436.500T^{-1}$

$\Delta Gf^\circ = 121.615 + 0.367\mathrm{x}10^{-3}T\ln T + 1.627\mathrm{x}10^{-6}T^2 - 218.250T^{-1} - 30.507\mathrm{x}10^{-3}T$

2130-2500 K: $\Delta Hf^\circ = 120.186 - 5.408\mathrm{x}10^{-3}T + 0.164\mathrm{x}10^{-6}T^2 - 450.100T^{-1}$

$\Delta Gf^\circ = 120.186 + 5.408\mathrm{x}10^{-3}T\ln T - 0.164\mathrm{x}10^{-6}T^2 - 225.050T^{-1} - 64.654\mathrm{x}10^{-3}T$

Source: Data from Chase (83) who estimated all except enthalpy of formation at 298 K.

$Cr_2N(c)$
Dichromium Nitride
[Formation: $2Cr(c,l) + 0.5N_2(g) = Cr_2N(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.790	15.500	15.500	0	-30.000	-24.429	17.907
300	15.820	15.598	15.501	.029	-29.998	-24.397	17.773
311.5	16.019	16.197	15.516	.212	-29.988	-24.182	16.966
400	17.550	20.408	16.143	1.706	-29.831	-22.551	12.321
500	18.340	24.412	17.410	3.501	-29.632	-20.751	9.070
600	19.000	27.814	18.867	5.368	-29.437	-18.992	6.918
700	19.660	30.792	20.362	7.301	-29.241	-17.264	5.390
800	20.310	33.460	21.835	9.300	-29.038	-15.567	4.253
900	20.970	35.890	23.263	11.364	-28.813	-13.895	3.374
1000	21.630	38.134	24.640	13.494	-28.575	-12.255	2.678
1100	22.290	40.226	25.962	15.690	-28.345	-10.631	2.112
1200	22.940	42.194	27.235	17.951	-28.132	-9.024	1.643
1300	23.600	44.056	28.458	20.278	-27.952	-7.456	1.253
1400	24.260	45.829	29.635	22.671	-27.788	-5.895	.920
1500	24.920	47.525	30.772	25.130	-27.636	-4.314	.629
1600	25.580	49.155	31.871	27.655	-27.512	-2.765	.378
1700	26.240	50.725	32.933	30.246	-27.411	-1.244	.160
1800	26.890	52.244	33.964	32.904	-27.325	.316	-.038
1900	27.430	53.712	34.965	35.619	-27.267	1.839	-.211
2000	28.080	55.136	35.939	38.395	-27.212	3.378	-.369
2100	28.670	56.520	36.886	41.232	-27.172	4.918	-.512
2130	28.859	56.928	37.165	42.095	-27.160	5.373	-.551
2130	28.859	56.928	37.165	42.095	-35.254	5.373	-.551
2200	29.300	57.868	37.808	44.131	-34.837	6.686	-.664
2300	29.860	59.183	38.710	47.089	-34.193	8.569	-.814
2400	30.420	60.466	39.590	50.103	-33.494	10.412	-.948
2500	31.000	61.719	40.449	53.174	-32.741	12.258	-1.072

*Entropy at 298 K estimated and data extrapolated above 800 K.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
2130 K, melting point of Cr; ΔH° = 4.047 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K:
$$Cp° = 15.879 + 6.060\times10^{-3}T - 1.685\times10^{5}T^{-2}$$
$$H° - H°_{298} = 15.879\times10^{-3}T + 3.030\times10^{-6}T^{2} + 1.685\times10^{2}T^{-1} - 5.569$$

Formation equations (kcal/mol):

298.15-311.5 K:
$$\Delta Hf° = -33.758 + 18.236\times10^{-3}T - 25.399\times10^{-6}T^{2} + 172.450T^{-1}$$
$$\Delta Gf° = -33.758 - 18.236\times10^{-3}T\ln T + 25.399\times10^{-6}T^{2} + 86.225T^{-1} + 126.651\times10^{-3}T$$
311.5-2000 K:
$$\Delta Hf° = -31.762 + 3.902\times10^{-3}T - 0.847\times10^{-6}T^{2} + 199.650T^{-1}$$
$$\Delta Gf° = -31.762 - 3.902\times10^{-3}T\ln T + 0.847\times10^{-6}T^{2} + 99.825T^{-1} + 45.455\times10^{-3}T$$
2000-2130 K:
$$\Delta Hf° = -30.425 + 2.838\times10^{-3}T - 0.580\times10^{-6}T^{2} - 350.300T^{-1}$$
$$\Delta Gf° = -30.425 - 2.838\times10^{-3}T\ln T + 0.580\times10^{-6}T^{2} - 175.150T^{-1} + 37.301\times10^{-3}T$$
2130-2500 K:
$$\Delta Hf° = -33.283 - 7.244\times10^{-3}T + 3.002\times10^{-6}T^{2} - 377.500T^{-1}$$
$$\Delta Gf° = -33.283 + 7.244\times10^{-3}T\ln T - 3.002\times10^{-6}T^{2} - 188.750T^{-1} - 30.992\times10^{-3}T$$

Source: Data from Chase (83) who estimated entropy at 298 K and extrapolated data above 800 K.

$Cr_2(SO_4)_3(c)$
Chromium Sulfate
[Reaction: $2Cr(c) + 1.5S_2(g) + 6O_2(g) = Cr_2(SO_4)_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	67.250	61.850	61.850	0	-751.065	-654.095	479.458
300*	67.458	62.267	61.850	.125	-751.059	-653.493	476.063
311.5	68.655	64.827	61.913	.908	-751.030	-649.753	455.864
400	77.864	83.137	64.627	7.404	-750.399	-621.051	339.322
500	86.643	101.485	70.199	15.643	-749.031	-588.852	257.384
600	93.796	117.939	76.807	24.679	-747.112	-556.986	202.880
700	99.322	132.834	83.765	34.348	-744.777	-525.476	164.059
800	103.222	146.369	90.758	44.489	-742.154	-494.329	135.043
900	105.495	158.674	97.632	54.938	-739.370	-463.517	112.556

*Data above 298 K estimated.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp° = 67.792 + 47.310\times10^{-3}T - 13.021\times10^{5}T^{-2}$
$H° - H°_{298} = 67.792\times10^{-3}T + 23.655\times10^{-6}T^{2} + 13.021\times10^{2}T^{-1} - 26.682$

Reaction equations (kcal/mol):

298.15-311.5 K: $\Delta Hr° = -758.692 + 17.513\times10^{-3}T - 7.977\times10^{-6}T^{2} + 928.450T^{-1}$
$\Delta Gr° = -758.692 - 17.513\times10^{-3}T\ln T + 7.977\times10^{-6}T^{2} + 464.225T^{-1} + 443.003\times10^{-3}T$
311.5-900 K: $\Delta Hr° = -756.696 + 3.179\times10^{-3}T + 16.575\times10^{-6}T^{2} + 955.650T^{-1}$
$\Delta Gr° = -756.696 - 3.179\times10^{-3}T\ln T - 16.575\times10^{-6}T^{2} + 477.825T^{-1} + 361.808\times10^{-3}T$

Source: Data from DeKock (112) who estimated all above 298 K.

$Cr_2(SO_4)_3\cdot 8H_2O(c)$
Chromium Sulfate Octahydrate
[Reaction: $2Cr(c) + 1.5S_2(g) + 10O_2(g) + 8H_2(g) = Cr_2(SO_4)_3\cdot 8H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	141.000	138.000	138.000	0	-1348.565	-1141.421	836.673
300	141.536	138.874	138.004	.261	-1348.579	-1140.136	830.578
311.5	144.871	144.261	138.136	1.908	-1348.644	-1132.144	794.307
350	156.036	161.781	139.778	7.701	-1348.720	-1105.377	690.220
400	170.536	183.563	143.901	15.865	-1347.986	-1070.674	584.981
450	185.036	204.486	149.477	24.754	-1346.746	-1036.073	503.179
500	199.536	224.732	155.994	34.369	-1344.869	-1001.647	437.814
550	214.036	244.430	163.143	44.708	-1342.357	-967.442	384.421

*Data except enthalpy of formation at 298 K estimated.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 54.024 + 290.934\times10^{-3}T + 0.209\times10^{5}T^{-2}$

$H°- H°_{298} = 54.024\times10^{-3}T + 145.467\times10^{-6}T^{2} - 0.209\times10^{2}T^{-1} - 28.968$

Reaction equations (kcal/mol):

298.15-311.5 K: $\Delta Hr° = -1333.816 - 76.823\times10^{-3}T + 108.471\times10^{-6}T^{2} - 443.350T^{-1}$

$\Delta Gr° = -1333.816 + 76.823\times10^{-3}T\ln T - 108.471\times10^{-6}T^{2} - 221.675T^{-1} + 242.426\times10^{-3}T$

311.5-550 K: $\Delta Hr° = -1331.820 - 91.157\times10^{-3}T + 133.023\times10^{-6}T^{2} - 416.150T^{-1}$

$\Delta Gr° = -1331.820 + 91.157\times10^{-3}T\ln T - 133.023\times10^{-6}T^{2} - 208.075T^{-1} + 161.231\times10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$Cr_2(SO_4)_3 \cdot 14H_2O(c)$
Chromium Sulfate Hydrate
[Reaction: $2Cr(c) + 1.5S_2(g) + 13O_2(g) + 14H_2(g) = Cr_2(SO_4)_3 \cdot 14H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	197.000	195.000	195.000	0	-1778.065	-1488.257	1090.907
300	197.925	196.221	195.004	.365	-1778.092	-1486.459	1082.871
311.5	203.675	203.774	195.190	2.674	-1778.214	-1475.277	1035.048
350	222.925	228.609	197.503	10.887	-1778.286	-1437.823	897.805
400	247.925	260.009	203.364	22.658	-1777.104	-1389.269	759.052
450	272.925	290.653	211.366	35.679	-1774.917	-1340.906	651.225
500	297.925	320.703	220.803	49.950	-1771.586	-1292.850	565.097
550	322.925	350.271	231.231	65.472	-1767.113	-1245.184	494.784

*Data except enthalpy of formation at 298 K estimated.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 47.436 + 500.902\times10^{-3}T + 0.196\times10^{5}T^{-2}$

$H°-H°_{298} = 47.436\times10^{-3}T + 250.451\times10^{-6}T^{2} - 0.196\times10^{2}T^{-1} - 36.341$

Reaction equations (kcal/mol):

298.15-311.5 K: $\Delta Hr° = -1752.192 - 143.837\times10^{-3}T + 209.432\times10^{-6}T^{2} - 478.650T^{-1}$

$\Delta Gr° = -1752.192 + 143.837\times10^{-3}T\ln T - 209.432\times10^{-6}T^{2} - 239.325T^{-1} + 130.855\times10^{-3}T$

311.5-550 K: $\Delta Hr° = -1750.197 - 158.170\times10^{-3}T + 233.984\times10^{-6}T^{2} - 451.450T^{-1}$

$\Delta Gr° = -1750.197 + 158.170\times10^{-3}T\ln T - 233.984\times10^{-6}T^{2} - 225.725T^{-1} + 49.660\times10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$Cr_2(SO_4)_3 \cdot 15H_2O(c)$

Chromium Sulfate Hydrate

[Reaction: $2Cr(c) + 1.5S_2(g) + 13.5O_2(g) + 15H_2(g) = Cr_2(SO_4)_3 \cdot 15H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	206.000	204.000	204.000	0	-1848.165	-1544.430	1132.083
300	206.999	205.277	204.004	.382	-1848.194	-1542.546	1123.730
311.5	213.209	213.180	204.197	2.798	-1848.329	-1530.827	1074.021
350	233.999	239.214	206.623	11.407	-1848.408	-1491.571	931.367
400	260.999	272.223	212.768	23.782	-1847.149	-1440.683	787.142
450	287.999	304.523	221.174	37.507	-1844.788	-1390.000	675.068
500	314.999	336.264	231.100	52.582	-1841.186	-1339.648	585.552
550	341.999	367.553	242.086	69.007	-1836.348	-1289.719	512.481

*Data except enthalpy of formation at 298 K estimated.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 45.024 + 539.966 \times 10^{-3}T - 0.013 \times 10^{5}T^{-2}$
$H° - H°_{298} = 45.024 \times 10^{-3}T + 269.983 \times 10^{-6}T^{2} + 0.013 \times 10^{2}T^{-1} - 37.428$

Reaction equations (kcal/mol):

298.15-311.5 K: $\Delta Hr° = -1820.296 - 156.320 \times 10^{-3}T + 228.293 \times 10^{-6}T^{2} - 463.850T^{-1}$
$\Delta Gr° = -1820.296 + 156.320 \times 10^{-3}T\ln T - 228.293 \times 10^{-6}T^{2} - 231.925T^{-1} + 105.289 \times 10^{-3}T$
311.5-550 K: $\Delta Hr° = -1818.301 - 170.654 \times 10^{-3}T + 252.845 \times 10^{-6}T^{2} - 436.650T^{-1}$
$\Delta Gr° = -1818.301 + 170.654 \times 10^{-3}T\ln T - 252.845 \times 10^{-6}T^{2} - 218.325T^{-1} + 24.093 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$Cr_2(SO_4)_3 \cdot 16H_2O(c)$
Chromium Sulfate Hydrate
[Reaction: $2Cr(c) + 1.5S_2(g) + 14O_2(g) + 16H_2(g) = Cr_2(SO_4)_3 \cdot 16H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	216.000	214.000	214.000	0	-1917.365	-1600.002	1172.818
300	217.073	215.339	214.002	.401	-1917.395	-1598.033	1164.151
311.5	223.743	223.630	214.206	2.936	-1917.531	-1585.788	1112.582
350	246.073	250.979	216.753	11.979	-1917.578	-1544.774	964.588
400	275.073	285.731	223.211	25.008	-1916.191	-1491.612	814.968
450	304.073	319.804	232.055	39.487	-1913.607	-1438.677	698.708
500	333.073	353.342	242.512	55.415	-1909.687	-1386.104	605.858
550	362.073	386.448	254.095	72.794	-1904.431	-1333.990	530.072

*Data except enthalpy of formation at 298 K estimated.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K:

$$Cp° = 43.610 + 579.034 \times 10^{-3}T - 0.222 \times 10^{5}T^{-2}$$

$$H°-H°_{298} = 43.610 \times 10^{-3}T + 289.517 \times 10^{-6}T^{2} + 0.222 \times 10^{2}T^{-1} - 38.813$$

Reaction equations (kcal/mol):

298.15-311.5 K:

$$\Delta Hr° = -1887.799 - 167.805 \times 10^{-3}T + 247.157 \times 10^{-6}T^{2} - 449.050T^{-1}$$

$$\Delta Gr° = -1887.799 + 167.805 \times 10^{-3}T\ln T - 247.157 \times 10^{-6}T^{2} - 224.525T^{-1} + 85.408 \times 10^{-3}T$$

311.5-550 K:

$$\Delta Hr° = -1885.803 - 182.139 \times 10^{-3}T + 271.709 \times 10^{-6}T^{2} - 421.850T^{-1}$$

$$\Delta Gr° = -1885.803 + 182.139 \times 10^{-3}T\ln T - 271.709 \times 10^{-6}T^{2} - 210.925T^{-1} + 4.212 \times 10^{-3}T$$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$Cr_2(SO_4)_3{\cdot}17H_2O(c)$
Chromium Sulfate Hydrate
[Reaction: $2Cr(c) + 1.5S_2(g) + 14.5O_2(g) + 17H_2(g) = Cr_2(SO_4)_3{\cdot}17H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	225.000	233.000	233.000	0	-1986.765	-1658.457	1215.666
300	226.128	234.395	233.005	.417	-1986.798	-1656.421	1206.686
311.5	233.143	243.033	233.217	3.058	-1986.948	-1643.753	1153.250
350	256.629	271.544	235.870	12.486	-1987.012	-1601.322	999.898
400	287.129	307.803	242.603	26.080	-1985.588	-1546.320	844.859
450	317.629	343.382	251.829	41.199	-1982.895	-1491.555	724.389
500	348.129	378.426	262.740	57.843	-1978.791	-1437.168	628.177
550	378.629	413.037	274.833	76.012	-1973.283	-1383.262	549.650

*Data except enthalpy of formation at 298 K estimated.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp^\circ = 43.153 + 609.966\times10^{-3}T - 0.013\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 43.153\times10^{-3}T + 304.983\times10^{-6}T^{2} + 0.013\times10^{2}T^{-1} - 39.981$

Reaction equations (kcal/mol):

298.15-311.5 K: $\Delta Hr^\circ = -1955.284 - 178.332\times10^{-3}T + 261.952\times10^{-6}T^{2} - 476.050T^{-1}$

$\Delta Gr^\circ = -1955.284 + 178.332\times10^{-3}T\ln T - 261.952\times10^{-6}T^{2} - 238.025T^{-1} + 60.277\times10^{-3}T$

311.5-550 K: $\Delta Hr^\circ = -1953.289 - 192.667\times10^{-3}T + 286.505\times10^{-6}T^{2} - 448.850T^{-1}$

$\Delta Gr^\circ = -1953.289 + 192.667\times10^{-3}T\ln T - 286.505\times10^{-6}T^{2} - 224.425T^{-1} - 20.919\times10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$CrSb_2$(c,l)
Chromium Diantimonide
[Formation: Cr(c) + 2Sb(c,l) = $CrSb_2$(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	19.660	27.460	27.460	0	-4.450	-4.465	3.273
300	19.680	27.580	27.460	.036	-4.446	-4.464	3.252
311.5	19.765	28.322	27.478	.263	-4.425	-4.465	3.133
400	20.420	33.350	28.245	2.042	-4.245	-4.501	2.459
500	20.800	37.950	29.736	4.107	-4.056	-4.581	2.002
600	20.860	41.750	31.433	6.190	-3.911	-4.709	1.715
700	21.200	44.990	33.147	8.290	-3.816	-4.845	1.513
800	21.720	47.850	34.806	10.435	-3.755	-5.003	1.367
900	22.260	50.440	36.401	12.635	-3.725	-5.156	1.252
903.9	22.280	50.538	36.463	12.722	-3.725	-5.163	1.248
903.9	22.280	50.538	36.463	12.722	-13.225	-5.163	1.248
904	22.280	50.540	36.463	12.724	-13.225	-5.156	1.246
904	22.280	50.610	36.463	12.790	-13.159	-5.156	1.246
991.3	22.810	52.680	37.792	14.760	-13.153	-4.390	.968
991.3	33.090	61.080	37.792	23.083	-4.830	-4.390	.968
1000	34.000	61.370	37.996	23.374	-4.736	-4.386	.959
1050	40.420	63.180	39.154	25.227	-4.021	-4.376	.911

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.
904 K, $CrSb_2$(c) to $CrSb_2$(c) + Sb(1); ΔH° = 0.066 kcal/mol.
991.3 K, peritectic decomposition point of $CrSb_2$; ΔH° = 8.323 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-904 K: $Cp° = 19.686 + 2.634\times10^{-3}T - 0.721\times10^{5}T^{-2}$
$H°-H°_{298} = 19.686\times10^{-3}T + 1.317\times10^{-6}T^{2} + 0.721\times10^{2}T^{-1} - 6.228$
904-991.3 K: $Cp° = -833.431 + 903.284\times10^{-3}T$
$H°-H°_{298} = -833.431\times10^{-3}T + 451.642\times10^{-6}T^{2} + 397.123$
991.3-1050 K: $Cp° = 36.930 - 0.402\times10^{-3}T$
$H°-H°_{298} = 36.930\times10^{-3}T - 0.201\times10^{-6}T^{2} - 13.328$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -7.168 + 12.318\times10^{-3}T - 15.094\times10^{-6}T^{2} + 115.300T^{-1}$
$\Delta Gf° = -7.168 - 12.318\times10^{-3}T\ln T + 15.094\times10^{-6}T^{2} + 57.650T^{-1} + 74.099\times10^{-3}T$
311.5-903.9 K: $\Delta Hf° = -6.170 + 5.151\times10^{-3}T - 2.818\times10^{-6}T^{2} + 128.900T^{-1}$
$\Delta Gf° = -6.170 - 5.151\times10^{-3}T\ln T + 2.818\times10^{-6}T^{2} + 64.450T^{-1} + 33.501\times10^{-3}T$
903.9-904 K: $\Delta Hf° = -13.177 + 0.327\times10^{-3}T - 0.474\times10^{-6}T^{2} + 85.700T^{-1}$
$\Delta Gf° = -13.177 - 0.327\times10^{-3}T\ln T + 0.474\times10^{-6}T^{2} + 42.850T^{-1} + 10.563\times10^{-3}T$
904-991.3 K: $\Delta Hf° = 390.174 - 852.790\times10^{-3}T + 449.851\times10^{-6}T^{2} + 13.600T^{-1}$
$\Delta Gf° = 390.174 + 852.790\times10^{-3}T\ln T - 449.851\times10^{-6}T^{2} + 6.800T^{-1} - 5835.505\times10^{-3}T$
991.3-1050 K: $\Delta Hf° = -20.277 + 17.571\times10^{-3}T - 1.992\times10^{-6}T^{2} + 13.600T^{-1}$
$\Delta Gf° = -20.277 - 17.571\times10^{-3}T\ln T + 1.992\times10^{-6}T^{2} + 6.800T^{-1} + 135.272\times10^{-3}T$

Source: Data from Alles (7).

$CrSi(c)$
Chromium Silicide
[Formation: $Cr(c) + Si(c,l) = CrSi(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	10.780	10.760	10.760	0	-13.800	-13.982	10.249
300	10.810	10.830	10.763	.020	-13.799	-13.985	10.188
311.5	10.956	11.239	10.773	.145	-13.796	-13.992	9.817
400	12.080	14.150	11.200	1.180	-13.727	-14.055	7.679
500	12.700	16.920	12.080	2.420	-13.655	-14.145	6.183
600	13.110	19.270	13.087	3.710	-13.595	-14.249	5.190
700	13.430	21.320	14.120	5.040	-13.543	-14.362	4.484
800	13.700	23.130	15.130	6.400	-13.500	-14.476	3.955
900	13.950	24.760	16.116	7.780	-13.470	-14.604	3.546
1000	14.170	26.240	17.060	9.180	-13.450	-14.730	3.219
1100	14.380	27.600	17.955	10.610	-13.443	-14.862	2.953
1200	14.580	28.860	18.810	12.060	-13.461	-14.985	2.729
1300	14.780	30.040	19.632	13.530	-13.512	-15.124	2.543
1400	14.970	31.140	20.411	15.020	-13.588	-15.240	2.379
1500	15.160	32.180	21.167	16.520	-13.697	-15.362	2.238
1600	15.350	33.160	21.879	18.050	-13.827	-15.459	2.112
1687	15.515	33.981	22.488	19.388	-13.972	-15.546	2.014
1687	15.515	33.981	22.488	19.388	-26.054	-15.546	2.014
1700	15.540	34.100	22.576	19.590	-26.068	-15.460	1.987

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1700 K: $Cp^\circ = 12.590 + 1.774\times10^{-3}T - 1.952\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 12.590\times10^{-3}T + 0.887\times10^{-6}T^{2} + 1.952\times10^{2}T^{-1} - 4.487$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -15.819 + 9.719\times10^{-3}T - 13.531\times10^{-6}T^{2} + 96.700T^{-1}$
$\Delta Gf^\circ = -15.819 - 9.719\times10^{-3}T\ln T + 13.531\times10^{-6}T^{2} + 48.350T^{-1} + 56.959\times10^{-3}T$
311.5-1687 K: $\Delta Hf^\circ = -14.822 + 2.552\times10^{-3}T - 1.255\times10^{-6}T^{2} + 110.300T^{-1}$
$\Delta Gf^\circ = -14.822 - 2.552\times10^{-3}T\ln T + 1.255\times10^{-6}T^{2} + 55.150T^{-1} + 16.362\times10^{-3}T$
1687-1700 K: $\Delta Hf^\circ = -27.251 + 2.131\times10^{-3}T - 0.904\times10^{-6}T^{2} + 208.800T^{-1}$
$\Delta Gf^\circ = -27.251 - 2.131\times10^{-3}T\ln T + 0.904\times10^{-6}T^{2} + 104.400T^{-1} + 21.176\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Eremenko (140). Low-temperature heat capacities and entropy at 298 K from Kalishevich (227). High-temperature data from Kalishevich (231).

$CrSi_2(c,l)$
Chromium Disilicide
[Formation: $Cr(c) + 2Si(c,l) = CrSi_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	15.200	13.300	13.300	0	-23.300	-22.897	16.784
300	15.240	13.390	13.300	.030	-23.298	-22.893	16.677
311.5	15.402	13.966	13.304	.206	-23.300	-22.877	16.051
400	16.650	17.980	13.905	1.630	-23.293	-22.761	12.436
500	17.580	21.800	15.120	3.340	-23.297	-22.627	9.890
600	18.310	25.080	16.513	5.140	-23.299	-22.495	8.194
700	18.960	27.950	17.950	7.000	-23.308	-22.363	6.982
800	19.580	30.520	19.358	8.930	-23.300	-22.220	6.070
900	20.190	32.860	20.727	10.920	-23.280	-22.083	5.362
1000	20.810	35.020	22.060	12.960	-23.248	-21.948	4.797
1100	21.440	37.030	23.321	15.080	-23.188	-21.824	4.336
1200	22.090	38.930	24.555	17.250	-23.130	-21.714	3.955
1300	22.770	40.720	25.720	19.500	-23.051	-21.595	3.630
1400	23.460	42.430	26.851	21.810	-22.964	-21.480	3.353
1500	24.180	44.080	27.953	24.190	-22.856	-21.401	3.118
1600	24.930	45.660	29.010	26.640	-22.734	-21.310	2.911
1687	25.600	46.993	29.894	28.847	-22.597	-21.189	2.745
1687	25.600	46.993	29.894	28.847	-46,761	-21.189	2.745
1700	25.700	47.190	30.025	29.180	-46.722	-20.984	2.698
1730	25.930	47.650	30.336	29.950	-46.636	-20.547	2.596
1730	20.300	65.340	30.336	60.560	-16.026	-20.547	2.596
1800	20.300	66.140	31.707	61.980	-16.216	-20.698	2.513
1900	20.300	67.240	33.551	64.010	-16.521	-20.948	2.410

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.
1730 K, melting point of $CrSi_2$; ΔH° = 30.610 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1730 K: $Cp° = 14.922 + 6.178\times10^{-3}T - 1.393\times10^{5}T^{-2}$
$H°-H°_{298} = 14.922\times10^{-3}T + 3.089\times10^{-6}T^{2} + 1.393\times10^{2}T^{-1} - 5.191$
1730-1900 K: $Cp° = 20.300$
$H°-H°_{298} = 20.300\times10^{-3}T + 25.441$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -23.968 + 6.372\times10^{-3}T - 11.680\times10^{-6}T^{2} - 57.700T^{-1}$
$\Delta Gf° = -23.968 - 6.372\times10^{-3}T\ln T + 11.680\times10^{-6}T^{2} - 28.850T^{-1} + 36.738\times10^{-3}T$
311.5-1687 K: $\Delta Hf° = -22.970 - 0.795\times10^{-3}T + 0.596\times10^{-6}T^{2} - 44.100T^{-1}$
$\Delta Gf° = -22.970 + 0.795\times10^{-3}T\ln T - 0.596\times10^{-6}T^{2} - 22.050T^{-1} - 3.860\times10^{-3}T$
1687-1730 K: $\Delta Hf° = -47.829 - 1.637\times10^{-3}T + 1.298\times10^{-6}T^{2} + 152.900T^{-1}$
$\Delta Gf° = -47.829 + 1.637\times10^{-3}T\ln T - 1.298\times10^{-6}T^{2} + 76.450T^{-1} + 5.768\times10^{-3}T$
1730-1900 K: $\Delta Hf° = -17.197 + 3.741\times10^{-3}T - 1.791\times10^{-6}T^{2} + 13.600T^{-1}$
$\Delta Gf° = -17.197 - 3.741\times10^{-3}T\ln T + 1.791\times10^{-6}T^{2} + 6.800T^{-1} + 22.839\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Eremenko (140). Other data based on Kalishevich (228).

$Cr_3Si(c)$
Trichromium Silicide
[Formation: $3Cr(c) + Si(c) = Cr_3Si(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	21.580	20.700	20.700	0	-30.000	-29.776	21.826
300	21.630	20.830	20.700	.040	-29.999	-29.777	21.692
311.5	21.881	21.648	20.717	.290	-30.005	-29.768	20.885
400	23.810	27.370	21.570	2.320	-29.969	-29.705	16.230
500	25.480	32.870	23.290	4.790	-29.911	-29.636	12.954
600	26.950	37.650	25.300	7.410	-29.837	-29.591	10.778
700	28.330	41.910	27.381	10.170	-29.729	-29.561	9.229
800	29.650	45.780	29.442	13.070	-29.570	-29.546	8.071
900	30.950	49.340	31.451	16.100	-29.350	-29.548	7.175
1000	32.220	52.670	33.410	19.260	-29.074	-29.584	6.465

Phase changes: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 20.109 + 12.308x10^{-3}T - 1.956x10^{5}T^{-2}$
$H°- H°_{298} = 20.109x10^{-3}T + 6.154x10^{-6}T^{2} + 1.956x10^{2}T^{-1} - 7.199$

Formation equations (kcal/mol):

298.15-311.5 K: $ΔHf° = -33.904 + 22.854x10^{-3}T - 36.398x10^{-6}T^{2} + 97.100T^{-1}$
$ΔGf° = -33.904 - 22.854x10^{-3}TlnT + 36.398x10^{-6}T^{2} + 48.550T^{-1} + 132.659x10^{-3}T$
311.5-1000 K: $ΔHf° = -30.911 + 1.353x10^{-3}T + 0.430x10^{-6}T^{2} + 137.900T^{-1}$
$ΔGf° = -30.911 - 1.353x10^{-3}TlnT - 0.430x10^{-6}T^{2} + 68.950T^{-1} + 10.866x10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Eremenko (140). Low-temperature heat capacities and entropy at 298 K from Surikov (487). High-temperature data based on Golutvin (176).

Cr_5Si_3(c,l)
Pentachromium Trisilicide
[Formation: $5Cr(c) + 3Si(c,l) = Cr_5Si_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	44.080	43.500	43.500	0	-61.000	-61.522	45.096
300	44.180	43.770	43.503	.080	-60.997	-61.531	44.825
311.5	44.673	45.441	43.544	.591	-60.987	-61.550	43.183
400	48.470	57.140	45.290	4.740	-60.763	-61.743	33.734
500	51.170	68.270	48.810	9.730	-60.521	-62.006	27.102
600	53.080	77.770	52.853	14.950	-60.307	-62.317	22.699
700	54.520	86.070	57.027	20.330	-60.135	-62.669	19.566
800	55.660	93.430	61.130	25.840	-60.000	-63.040	17.222
900	56.680	100.040	65.084	31.460	-59.890	-63.418	15.400
1000	57.720	106.070	68.890	37.180	-59.814	-63.804	13.944
1100	58.900	111.620	72.520	43.010	-59.825	-64.214	12.758
1200	60.360	116.810	76.002	48.970	-59.917	-64.597	11.765
1300	62.230	121.710	79.333	55.090	-60.102	-65.029	10.932
1400	64.620	126.410	82.531	61.430	-60.278	-65.416	10.212
1500	67.670	130.960	85.600	68.040	-60.387	-65.742	9.578
1600	71.500	135.450	88.581	74.990	-60.401	-66.113	9.030
1687	75.624	139.337	91.096	81.383	-60.253	-66.416	8.604
1687	75.624	139.337	91.096	81.383	-96.499	-66.416	8.604
1700	76.240	139.920	91.467	82.370	-96.432	-66.172	8.507
1800	82.000	144.440	94.290	90.270	-95.732	-64.358	7.814
1900	88.910	149.050	97.045	98.810	-94.597	-62.658	7.207
1920	90.440	149.990	97.592	100.600	-94.304	-62.325	7.094
1920	120.000	181.600	97.592	161.300	-33.604	-62.325	7.094
2000	120.000	186.500	101.050	170.900	-30.067	-63.587	6.948

Phase change:
311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.
1920 K, melting point of Cr_5Si_3; ΔH° = 60.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1920 K: $C_p^\circ = 40.363 + 19.842\times10^{-3}T - 1.956\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 40.363\times10^{-3}T + 9.921\times10^{-6}T^{2} + 1.956\times10^{2}T^{-1} - 13.572$
1920-2100 K: $C_p^\circ = 120.000$
$H^\circ - H^\circ_{298} = 120.000\times10^{-3}T - 69.100$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -66.342 + 37.366\times10^{-3}T - 61.467\times10^{-6}T^{2} - 99.900T^{-1}$
$\Delta Gf^\circ = -66.342 - 37.366\times10^{-3}T\ln T + 61.467\times10^{-6}T^{2} - 49.950T^{-1} + 211.298\times10^{-3}T$
311.5-1687 K: $\Delta Hf^\circ = -61.353 + 1.531\times10^{-3}T - 0.087\times10^{-6}T^{2} - 31.900T^{-1}$
$\Delta Gf^\circ = -61.353 - 1.531\times10^{-3}T\ln T + 0.087\times10^{-6}T^{2} - 15.950T^{-1} + 8.310\times10^{-3}T$
1687-1920 K: $\Delta Hf^\circ = -98.640 + 0.268\times10^{-3}T + 0.966\times10^{-6}T^{2} + 263.600T^{-1}$
$\Delta Gf^\circ = -98.640 - 0.268\times10^{-3}T\ln T - 0.966\times10^{-6}T^{2} + 131.800T^{-1} + 22.752\times10^{-3}T$
1920-2000 K: $\Delta Hf^\circ = -154.169 + 79.905\times10^{-3}T - 8.955\times10^{-6}T^{2} + 68.000T^{-1}$
$\Delta Gf^\circ = -154.169 - 79.905\times10^{-3}T\ln T + 8.955\times10^{-6}T^{2} + 34.000T^{-1} + 634.713\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Eremenko (140). Other data based on Kalishevich (228).

$(Cs_{0.650}Na_{0.185}Rb_{0.028})(AlSi_2)(O_{5.863}[OH]_{0.137})\cdot 0.19H_2O(c)$

Pollucite

[Formation: $0.65Cs(c,l) + 0.185Na(c,l) + 0.028Rb(c,l) + Al(c) + 2Si(c)$
$+ 3.095O_2(g) + 0.259H_2(g) = \text{pollucite}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	41.562	49.531	49.531	0	-740.564	-698.219	511.801
300	41.631	49.789	49.532	.077	-740.571	-697.955	508.454
301.55	41.691	50.004	49.534	.142	-740.577	-697.735	505.681
301.55	41.691	50.004	49.534	.142	-740.902	-697.735	505.681
312.64	42.117	51.517	49.578	.606	-740.943	-696.147	486.633
312.64	42.117	51.517	49.578	.606	-740.957	-696.147	486.633
350	43.552	56.349	50.046	2.206	-741.080	-690.790	431.343
371	44.406	58.912	50.476	3.130	-741.134	-687.770	405.149
371	44.406	58.912	50.476	3.130	-741.249	-687.770	405.149
400	45.585	62.296	51.211	4.434	-741.309	-683.587	373.490
450	47.694	67.786	52.750	6.766	-741.361	-676.365	328.483
500	49.824	72.920	54.514	9.203	-741.345	-669.143	292.478
550	51.990	77.771	56.411	11.748	-741.258	-661.928	263.023
600	54.175	82.388	58.383	14.403	-741.095	-654.722	238.479
650	56.372	86.811	60.402	17.166	-740.859	-647.534	217.718
675	57.474	88.959	61.420	18.589	-740.711	-643.947	208.493

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
312.64 K, melting point of Rb; ΔH° = 0.524 kcal/mol.
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-675 K: $Cp° = 27.038 + 44.730\times10^{-3}T + 1.056\times10^{5}T^{-2}$
$H°- H°_{298} = 27.038\times10^{-3}T + 22.365\times10^{-6}T^{2} - 1.056\times10^{2}T^{-1} - 9.695$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -735.535 - 15.745\times10^{-3}T + 12.115\times10^{-6}T^{2} - 420.821T^{-1}$
$\Delta Gf° = -735.535 + 15.745\times10^{-3}T\ln T - 12.115\times10^{-6}T^{2} - 210.410T^{-1} + 41.429\times10^{-3}T$
301.55-312.64 K: $\Delta Hf° = -735.628 - 18.343\times10^{-3}T + 17.011\times10^{-6}T^{2} - 388.776T^{-1}$
$\Delta Gf° = -735.628 + 18.343\times10^{-3}T\ln T - 17.011\times10^{-6}T^{2} - 194.388T^{-1} + 28.206\times10^{-3}T$
312.64-371 K: $\Delta Hf° = -735.618 - 18.549\times10^{-3}T + 17.352\times10^{-6}T^{2} - 386.726T^{-1}$
$\Delta Gf° = -735.618 + 18.549\times10^{-3}T\ln T - 17.352\times10^{-6}T^{2} - 193.363T^{-1} + 27.091\times10^{-3}T$
371-675 K: $\Delta Hf° = -735.690 - 19.114\times10^{-3}T + 18.231\times10^{-6}T^{2} - 369.909T^{-1}$
$\Delta Gf° = -735.690 + 19.114\times10^{-3}T\ln T - 18.231\times10^{-6}T^{2} - 184.955T^{-1} + 24.208\times10^{-3}T$

Source: Data from Bennington (29).

$Cs_2CO_3(c)$
Cesium Carbonate
[Formation: $2Cs(c,l,g) + C(c) + 1.5O_2(g) = Cs_2CO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	29.600	48.870	48.870	0	-271.250	-251.349	184.241
300*	29.650	49.050	48.870	.055	-271.247	-251.223	183.014
301.55	29.695	49.203	48.868	.101	-271.244	-251.120	181.998
301.55	29.695	49.203	48.868	.101	-272.244	-251.120	181.998
400	32.580	58.010	50.072	3.175	-271.960	-244.262	133.457
500	34.830	65.530	52.432	6.549	-271.497	-237.389	103.761
600	36.800	72.060	55.173	10.132	-270.908	-230.620	84.002
700	38.650	77.870	58.004	13.906	-270.204	-223.957	69.922
800	40.440	83.150	60.824	17.861	-269.385	-217.409	59.393
900	42.180	88.010	63.574	21.992	-268.440	-210.963	51.228
952	43.080	90.410	64.982	24.208	-267.898	-207.688	47.678
952	43.080	90.410	64.982	24.208	-300.294	-207.688	47.678
1000	43.910	92.550	66.254	26.296	-299.526	-203.038	44.373

*Data above 298 K estimated.

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K:

$$Cp° = 27.591 + 16.570\times10^{-3}T - 2.620\times10^{5}T^{-2}$$

$$H°-H°_{298} = 27.591\times10^{-3}T + 8.285\times10^{-6}T^{2} + 2.620\times10^{2}T^{-1} - 9.841$$

Formation equations (kcal/mol):

298.15-301.55 K:

$$\Delta Hf° = -272.639 + 6.956\times10^{-3}T - 8.530\times10^{-6}T^{2} + 21.900T^{-1}$$

$$\Delta Gf° = -272.639 - 6.956\times10^{-3}T\ln T + 8.530\times10^{-6}T^{2} + 10.950T^{-1} + 108.375\times10^{-3}T$$

301.55-952 K:

$$\Delta Hf° = -272.925 - 1.038\times10^{-3}T + 6.535\times10^{-6}T^{2} + 120.500T^{-1}$$

$$\Delta Gf° = -272.925 + 1.038\times10^{-3}T\ln T - 6.535\times10^{-6}T^{2} + 60.250T^{-1} + 67.687\times10^{-3}T$$

952.00-1000 K:

$$\Delta Hf° = -309.996 + 3.710\times10^{-3}T + 6.636\times10^{-6}T^{2} + 179.700T^{-1}$$

$$\Delta Gf° = -309.996 - 3.710\times10^{-3}T\ln T - 6.636\times10^{-6}T^{2} + 89.850T^{-1} + 139.256\times10^{-3}T$$

Source: Data from Chang (74) who estimated all above 298 K.

Cs_2CrO_4(c,l)
Cesium Chromate
[Formation: $2Cs(c,l,g) + Cr(c) + 2O_2(g) = Cs_2CrO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	34.910	54.630	54.630	0	-341.780	-315.015	230.909
300	34.982	54.846	54.630	.065	-341.779	-314.849	229.364
301.55	35.031	55.026	54.631	.119	-341.779	-314.709	228.084
301.55	35.031	55.026	54.631	.119	-342.779	-314.709	228.084
311.5	35.347	56.169	54.662	.469	-342.781	-313.783	220.149
400	38.160	65.384	56.047	3.735	-342.634	-305.561	166.949
500	40.747	74.182	58.818	7.682	-342.269	-296.330	129.524
600	43.092	81.821	62.028	11.876	-341.727	-287.188	104.607
700	45.443	88.636	65.350	16.300	-341.026	-278.149	86.841
800	48.752	94.901	68.656	20.996	-340.118	-269.229	73.549
900	54.867	100.957	71.909	26.143	-338.807	-260.440	63.243
952	60.967	104.144	73.583	29.093	-337.870	-255.964	58.761
952	60.967	104.144	73.583	29.093	-370.266	-255.964	58.761
1000	66.598	107.281	75.126	32.155	-368.843	-250.236	54.688
1031	71.942	109.393	76.124	34.300	-367.763	-246.575	52.268
1031	49.968	110.072	76.124	35.000	-367.063	-246.575	52.268
1100	51.730	113.365	78.357	38.509	-365.947	-238.544	47.394
1200	54.283	117.976	81.468	43.809	-364.159	-227.035	41.348
1236	55.203	119.593	82.554	45.780	-363.469	-222.930	39.418
1236	50.420	126.519	82.555	54.340	-354.909	-222.930	39.418
1300	50.420	129.065	84.783	57.567	-353.978	-216.130	36.334
1400	50.420	132.801	88.080	62.609	-352.569	-205.584	32.093
1500	50.420	136.280	91.179	67.651	-351.207	-195.123	28.429

Phase changes:
301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
311.5 K, second order transition of Cr: ΔH° = 0 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.
1031 K, transition point of Cs_2CrO_4; ΔH° = 0.700 kcal/mol.
1236 K, melting point of Cs_2CrO_4; ΔH° = 8.560 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1031 K: $Cp° = 17.787 + 41.608\times10^{-3}T + 4.193\times10^{5}T^{-2}$
$H°-H°_{298} = 17.787\times10^{-3}T + 20.804\times10^{-6}T^{2} - 4.193\times10^{2}T^{-1} - 5.746$
1031-1236 K: $Cp° = 23.644 + 25.534\times10^{-3}T$
$H°-H°_{298} = 23.644\times10^{-3}T + 12.767\times10^{-6}T^{2} - 2.948$
1236-1500 K: $Cp° = 50.420$
$H°-H°_{298} = 50.420\times10^{-3}T - 7.979$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -339.180 - 0.137\times10^{-3}T - 9.563\times10^{-6}T^{2} - 509.700T^{-1}$
$\Delta Gf° = -339.180 + 0.137\times10^{-3}T\ln T + 9.563\times10^{-6}T^{2} - 254.850T^{-1} + 80.283\times10^{-3}T$
301.55-311.5 K: $\Delta Hf° = -339.466 - 8.131\times10^{-3}T + 5.501\times10^{-6}T^{2} - 411.100T^{-1}$
$\Delta Gf° = -339.466 + 8.131\times10^{-3}T\ln T - 5.501\times10^{-6}T^{2} - 205.550T^{-1} + 39.596\times10^{-3}T$
311.5-952 K: $\Delta Hf° = -338.468 - 15.298\times10^{-3}T + 17.777\times10^{-6}T^{2} - 397.500T^{-1}$
$\Delta Gf° = -338.468 + 15.298\times10^{-3}T\ln T - 17.777\times10^{-6}T^{2} - 198.750T^{-1} - 1.002\times10^{-3}T$
952-1031 K: $\Delta Hf° = -375.539 - 10.550\times10^{-3}T + 17.879\times10^{-6}T^{2} - 338.300T^{-1}$
$\Delta Gf° = -375.539 + 10.550\times10^{-3}T\ln T - 17.879\times10^{-6}T^{2} - 169.150T^{-1} + 70.567\times10^{-3}T$
1031-1236 K: $\Delta Hf° = -372.741 - 4.693\times10^{-3}T + 9.842\times10^{-6}T^{2} + 81.000T^{-1}$
$\Delta Gf° = -372.741 + 4.693\times10^{-3}T\ln T - 9.842\times10^{-6}T^{2} + 40.500T^{-1} + 100.007\times10^{-3}T$
1236-1500 K: $\Delta Hf° = -377.772 + 22.083\times10^{-3}T - 2.925\times10^{-6}T^{2} + 81.000T^{-1}$
$\Delta Gf° = -377.772 - 22.083\times10^{-3}T\ln T + 2.925\times10^{-6}T^{2} + 40.500T^{-1} + 278.933\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from O'Hare (365). Low-temperature heat capacities and entropy at 298 K from Lyon (312). High-temperature data based on Fredrickson (159).

$Cs_3CrO_4(c)$
Tricesium Chromium Tetroxide
[Formation: $3Cs(c,l,g) + Cr(c) + 2O_2(g) = Cs_3CrO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	43.000	70.791	70.791	0	-368.820	-340.800	249.810
300	43.090	71.056	70.793	.079	-368.819	-340.626	248.143
301.55	43.153	71.278	70.795	.146	-368.819	-340.481	246.762
301.55	43.153	71.278	70.795	.146	-370.319	-340.481	246.762
311.5	43.555	72.686	70.833	.577	-370.316	-339.496	238.189
400	47.130	83.999	72.527	4.589	-370.096	-330.762	180.718
500	51.460	94.976	75.946	9.515	-369.501	-320.990	140.303
600	56.021	104.759	79.946	14.888	-368.522	-311.370	113.415
700	60.851	113.752	84.139	20.729	-367.144	-301.945	94.270
774	64.591	120.052	87.273	25.371	-365.848	-295.121	83.331
774	53.322	120.608	87.273	25.801	-365.418	-295.121	83.331
800	53.870	122.378	88.385	27.194	-365.207	-292.763	79.978
900	55.951	128.843	92.527	32.684	-364.292	-283.759	68.905
952	57.021	132.016	94.599	35.621	-363.754	-279.160	64.086
952	57.021	132.016	94.599	35.621	-412.348	-279.160	64.086
1000	58.009	134.845	96.463	38.382	-411.463	-272.466	59.547

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
774 K, transition point of Cs_3CrO_4; ΔH° = 0.430 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-774 K: $Cp° = 26.594 + 48.438\times10^{-3}T + 1.746\times10^{5}T^{-2}$
$H°-H°_{298} = 26.594\times10^{-3}T + 24.219\times10^{-6}T^{2} - 1.746\times10^{2}T^{-1} - 9.496$
774-1000 K: $Cp° = 37.218 + 20.802\times10^{-3}T$
$H°-H°_{298} = 37.218\times10^{-3}T + 10.401\times10^{-6}T^{2} - 9.237$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -368.355 + 5.534\times10^{-3}T - 13.795\times10^{-6}T^{2} - 265.000T^{-1}$
$\Delta Gf° = -368.355 - 5.534\times10^{-3}T\ln T + 13.795\times10^{-6}T^{2} - 132.500T^{-1} + 121.327\times10^{-3}T$
301.55-311.5 K: $\Delta Hf° = -368.784 - 6.457\times10^{-3}T + 8.801\times10^{-6}T^{2} - 117.100T^{-1}$
$\Delta Gf° = -368.784 + 6.457\times10^{-3}T\ln T - 8.801\times10^{-6}T^{2} - 58.550T^{-1} + 60.295\times10^{-3}T$
311.5-774 K: $\Delta Hf° = -367.786 - 13.624\times10^{-3}T + 21.077\times10^{-6}T^{2} - 103.500T^{-1}$
$\Delta Gf° = -367.786 + 13.624\times10^{-3}T\ln T - 21.077\times10^{-6}T^{2} - 51.750T^{-1} + 19.698\times10^{-3}T$
774-952 K: $\Delta Hf° = -367.527 - 3.000\times10^{-3}T + 7.259\times10^{-6}T^{2} + 71.100T^{-1}$
$\Delta Gf° = -367.527 + 3.000\times10^{-3}T\ln T - 7.259\times10^{-6}T^{2} + 35.550T^{-1} + 79.188\times10^{-3}T$
952-1000 K: $\Delta Hf° = -423.133 + 4.122\times10^{-3}T + 7.412\times10^{-6}T^{2} + 159.900T^{-1}$
$\Delta Gf° = -423.133 - 4.122\times10^{-3}T\ln T - 7.412\times10^{-6}T^{2} + 79.950T^{-1} + 186.541\times10^{-3}T$

Source: Data from Kim (255).

Cs_2MoO_4(c)
Cesium Molybdate
[Formation: $2Cs(c,l,g) + Mo(c,l) + 2O_2(g) = Cs_2MoO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	35.533	59.360	59.360	0	-362.000	-336.288	246.502
300	35.600	59.580	59.360	.066	-361.999	-336.127	244.865
301.55	35.651	59.764	59.362	.121	-361.998	-335.993	243.510
301.55	35.651	59.764	59.362	.121	-362.998	-335.993	243.510
400	38.875	70.291	60.799	3.797	-362.799	-327.200	178.771
500	41.758	79.279	63.619	7.830	-362.333	-318.349	139.148
600	44.505	87.136	66.896	12.144	-361.638	-309.612	112.775
700	47.188	94.199	70.300	16.729	-360.726	-301.009	93.978
800	49.837	100.673	73.698	21.580	-359.600	-292.557	79.922
845	51.022	103.432	75.208	23.850	-359.019	-288.800	74.694
845	44.256	104.817	75.208	25.020	-357.849	-288.800	74.694
900	45.710	107.654	77.105	27.494	-357.451	-284.318	69.041
952	47.084	110.259	78.844	29.907	-357.012	-280.129	64.308
952	47.084	110.259	78.844	29.907	-389.408	-280.129	64.308
1000	48.352	112.606	80.409	32.197	-388.714	-274.636	60.021
1100	50.995	117.339	83.554	37.164	-387.103	-263.303	52.313
1200	53.637	121.889	86.559	42.396	-385.257	-252.125	45.918

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
845 K, transition point of Cs_2MoO_4; ΔH° = 1.170 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-845 K: $Cp° = 29.356 + 25.860x10^{-3}T - 1.318x10^{5}T^{-2}$
$H°- H°_{298} = 29.356x10^{-3}T + 12.930x10^{-6}T^{2} + 1.318x10^{2}T^{-1} - 10.344$
845-1200 K: $Cp° = 21.927 + 26.424x10^{-3}T$
$H°- H°_{298} = 21.927x10^{-3}T + 13.212x10^{-6}T^{2} - 2.942$

Formation equations (kcal/mol):

298.15-301.55 K: $ΔHf° = -363.199 + 4.247x10^{-3}T - 4.555x10^{-6}T^{2} + 100.600T^{-1}$
$ΔGf° = -363.199 - 4.247x10^{-3}TlnT + 4.555x10^{-6}T^{2} + 50.300T-1+ 112.534x10^{-3}T$
301.55-845 K: $ΔHf° = -363.485 - 3.747x10^{-3}T + 10.509x10^{-6}T^{2} + 199.200T^{-1}$
$ΔGf° = -363.485 + 3.747x10^{-3}TlnT - 10.509x10^{-6}T^{2} + 99.600T^{-1} + 71.846x10^{-3}T$
845-952 K: $ΔHf° = -356.083 - 11.176x10^{-3}T + 10.791x10^{-6}T^{2} + 67.400T^{-1}$
$ΔGf° = -356.083 + 11.176x10^{-3}TlnT - 10.791x10^{-6}T^{2} + 33.700T^{-1} + 13.351x10^{-3}T$
952-1200 K: $ΔHf° = -393.154 - 6.428x10^{-3}T + 10.893x10^{-6}T^{2} + 126.600T^{-1}$
$ΔGf° = -393.154 + 6.428x10^{-3}TlnT - 10.893x10^{-6}T^{2} + 63.300T^{-1} + 84.919x10^{-3}T$

Sources: Enthalpy of formation at 298 K from O'Hare (368). Low-temperature heat capacities and entropy at 298 K from Osborne (379). High-temperature data based on Fredrickson (158) and Kohli (277).

$CsNO_3(c,l)$
Cesium Nitrate
[Formation: $Cs(c,l) + 0.5N_2(g) + 1.5O_2(g) = CsNO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.060	36.800	36.800	0	-120.880	-97.039	71.131
300	23.131	36.943	36.800	.043	-120.877	-96.890	70.584
301.55	23.208	37.062	36.801	.079	-120.875	-96.767	70.131
301.55	23.208	37.062	36.801	.079	-121.375	-96.767	70.131
400	28.581	44.299	37.766	2.613	-120.982	-88.777	48.505
425	30.479	46.087	38.204	3.350	-120.792	-86.770	44.620
425	33.020	48.169	38.204	4.235	-119.907	-86.770	44.620
500	34.505	53.645	40.119	6.763	-119.029	-80.995	35.403
600	37.427	60.178	42.926	10.351	-117.673	-73.511	26.776
679	40.498	64.986	45.214	13.425	-116.389	-67.773	21.814
679	40.724	69.949	45.214	16.795	-113.019	-67.773	21.814
700	41.226	71.197	45.976	17.655	-112.639	-66.380	20.725
750	43.638	74.113	47.754	19.769	-111.676	-63.111	18.390

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
425 K, transition point of $CsNO_3$; ΔH° = 0.885 kcal/mol.
679 K, melting point of $CsNO_3$; ΔH° = 3.370 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-425 K: $Cp° = -7.718 + 82.248x10^{-3}T + 5.562x10^{5}T^{-2}$
$H°- H°_{298} = -7.718x10^{-3}T + 41.124x10^{-6}T^{2} - 5.562x10^{2}T^{-1} + 0.511$
425-679 K: $Cp° = 5.895 + 46.534x10^{-3}T + 13.272x10^{5}T^{-2}$
$H°- H°_{298} = 5.895x10^{-3}T + 23.267x10^{-6}T^{2} - 13.272x10^{2}T^{-1} + 0.650$
679-750 K: $Cp° = 15.165 + 37.398x10^{-3}T$
$H°- H°_{298} = 15.165x10^{-3}T + 18.699x10^{-6}T^{2} - 2.123$

Formation equations (kcal/mol):

298.15-301.55 K: $ΔHf° = -114.242 - 24.958x10^{-3}T + 32.428x10^{-6}T^{2} - 620.050T^{-1}$
$ΔGf° = -114.242 + 24.958x10^{-3}TlnT - 32.428x10^{-6}T^{2} - 310.025T^{-1} - 71.344x10^{-3}T$
301.55-425 K: $ΔHf° = -114.385 - 28.955x10^{-3}T + 39.960x10^{-6}T^{2} - 570.750T^{-1}$
$ΔGf° = -114.385 + 28.955x10^{-3}TlnT - 39.960x10^{-6}T^{2} - 285.375T^{-1} - 91.687x10^{-3}T$
425-679 K: $ΔHf° = -114.246 - 15.342x10^{-3}T + 22.103x10^{-6}T^{2} - 1341.750T^{-1}$
$ΔGf° = -114.246 + 15.342x10^{-3}TlnT - 22.103x10^{-6}T^{2} - 670.875T^{-1} - 15.082x10^{-3}T$
679-750 K: $ΔHf° = -117.019 - 6.071x10^{-3}T + 17.535x10^{-6}T^{2} - 14.550T^{-1}$
$ΔGf° = -117.019 + 6.071x10^{-3}TlnT - 17.535x10^{-6}T^{2} - 7.275T^{-1} + 44.907x10^{-3}T$

Sources: Enthalpy of formation at 298 K from O'Hare (364). Low-temperature heat capacities and entropy at 298 K from Flotow (150). High-temperature data based on Flotow (150), Ichikawa (212), Mustajoki (342), and Stern (473).

CsOH(c,l)

Cesium Hydroxide

[Formation: $Cs(c,l,g) + 0.5H_2(g) + 0.5O_2(g) = CsOH(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.220	23.600	23.600	0	-99.600	-88.605	64.949
300	16.250	23.700	23.600	.030	-99.597	-88.537	64.498
301.55	16.274	23.784	23.601	.055	-99.595	-88.480	64.125
301.55	16.274	23.784	23.601	.055	-100.095	-88.480	64.125
400	17.780	28.589	24.257	1.733	-99.858	-84.719	46.288
410	17.840	29.026	24.367	1.910	-99.827	-84.341	44.957
410	18.800	29.782	24.367	2.220	-99.517	-84.341	44.957
493	18.800	33.248	25.581	3.780	-99.172	-81.302	36.041
493	19.700	36.189	25.581	5.230	-97.722	-81.302	36.041
500	19.700	36.467	25.727	5.370	-97.685	-81.067	35.434
588	20.100	39.698	27.581	7.125	-97.223	-78.179	29.058
588	19.500	41.552	27.581	8.215	-96.133	-78.179	29.058
600	19.500	41.946	27.864	8.449	-96.076	-77.814	28.343
700	19.500	44.952	30.096	10.399	-95.605	-74.807	23.356
800	19.500	47.556	32.120	12.349	-95.147	-71.869	19.633
900	19.500	49.853	33.965	14.299	-94.699	-68.986	16.752
952	19.500	50.949	34.864	15.313	-94.470	-67.519	15.500
952	19.500	50.949	34.864	15.313	-110.668	-67.519	15.500
1000	19.500	51.908	35.659	16.249	-110.342	-65.351	14.282
1100	19.500	53.766	37.221	18.199	-109.672	-60.884	12.096
1200	19.500	55.463	38.672	20.149	-109.010	-56.477	10.286

*Data estimated except enthalpy of formation at 298 K and temperatures and enthalpies of transitions and fusion.

Phase changes:
301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
410 K, α - β transition point of CsOH; ΔH° = 0.310 kcal/mol.
493 K, β - γ transition point of CsOH; ΔH° = 1.450 kcal/mol.
588 K, melting point of CsOH; ΔH° = 1.090 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-410 K: $Cp° = 17.720 + 3.260\text{x}10^{-3}T - 2.197\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 17.720\text{x}10^{-3}T + 1.630\text{x}10^{-6}T^2 + 2.197\text{x}10^{2}T^{-1} - 6.165$
410-493 K: $Cp° = 18.800$
$H°-H°_{298} = 18.800\text{x}10^{-3}T - 5.488$
493-588 K: $Cp° = 17.132 + 5.208\text{x}10^{-3}T$
$H°-H°_{298} = 17.132\text{x}10^{-3}T + 2.604\text{x}10^{-6}T^2 - 3.849$
588-1200 K: $Cp° = 19.500$
$H°-H°_{298} = 19.500\text{x}10^{-3}T - 3.251$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -102.021 + 7.741\text{x}10^{-3}T - 6.478\text{x}10^{-6}T^2 + 205.350T^{-1}$
$\Delta Gf° = -102.021 - 7.741\text{x}10^{-3}T\ln T + 6.478\text{x}10^{-6}T^2 + 102.675T^{-1} + 86.014\text{x}10^{-3}T$
301.55-410 K: $\Delta Hf° = -102.164 + 3.744\text{x}10^{-3}T + 1.054\text{x}10^{-6}T^2 + 254.650T^{-1}$
$\Delta Gf° = -102.164 - 3.744\text{x}10^{-3}T\ln T - 1.054\text{x}10^{-6}T^2 + 127.325T^{-1} + 65.670\text{x}10^{-3}T$
410-493 K: $\Delta Hf° = -101.487 + 4.824\text{x}10^{-3}T - 0.576\text{x}10^{-6}T^2 + 34.950T^{-1}$
$\Delta Gf° = -101.487 - 4.824\text{x}10^{-3}T\ln T + 0.576\text{x}10^{-6}T^2 + 17.475T^{-1} + 70.502\text{x}10^{-3}T$
493-588 K: $\Delta Hf° = -99.847 + 3.156\text{x}10^{-3}T + 2.028\text{x}10^{-6}T^2 + 34.950T^{-1}$
$\Delta Gf° = -99.847 - 3.156\text{x}10^{-3}T\ln T - 2.028\text{x}10^{-6}T^2 + 17.475T^{-1} + 58.118\text{x}10^{-3}T$
588-952 K: $\Delta Hf° = -99.250 + 5.524\text{x}10^{-3}T - 0.576\text{x}10^{-6}T^2 + 34.950T^{-1}$
$\Delta Gf° = -99.250 - 5.524\text{x}10^{-3}T\ln T + 0.576\text{x}10^{-6}T^2 + 17.475T^{-1} + 70.670\text{x}10^{-3}T$
952-1200 K: $\Delta Hf° = -117.785 + 7.898\text{x}10^{-3}T - 0.525\text{x}10^{-6}T^2 + 64.550T^{-1}$
$\Delta Gf° = -117.785 - 7.898\text{x}10^{-3}T\ln T + 0.525\text{x}10^{-6}T^2 + 32.275T^{-1} + 106.454\text{x}10^{-3}T$

Source: Data from Chase (81) who estimated all except enthalpy of formation at 298 K and temperatures and enthalpies of transitions and fusion.

CsOH(g)
Cesium Hydroxide (ideal gas)
[Formation: Cs(c,l,g) + $0.5H_2(g)$ + $0.5O_2(g)$ = CsOH(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.884	60.866	60.866	0	-62.000	-62.116	45.532
300	11.895	60.940	60.867	.022	-62.005	-62.117	45.251
301.55	11.902	61.001	60.867	.040	-62.009	-62.117	45.019
301.55	11.902	61.001	60.867	.040	-62.509	-62.117	45.019
400	12.315	64.427	61.340	1.235	-62.756	-61.952	33.849
500	12.529	67.200	62.244	2.478	-62.977	-61.726	26.980
600	12.665	69.497	63.267	3.738	-63.187	-61.455	22.385
700	12.777	71.458	64.299	5.011	-63.393	-61.149	19.091
800	12.886	73.171	65.303	6.294	-63.603	-60.816	16.614
900	12.999	74.695	66.264	7.588	-63.810	-60.454	14.680
952	13.060	75.427	66.745	8.266	-63.918	-60.270	13.836
952	13.060	75.427	66.745	8.266	-80.116	-60.270	13.836
1000	13.116	76.071	67.177	8.894	-80.097	-59.269	12.953
1100	13.234	77.326	68.043	10.211	-80.060	-57.188	11.362
1200	13.350	78.483	68.866	11.540	-80.019	-55.110	10.037
1300	13.462	79.556	69.648	12.881	-79.976	-53.035	8.916
1400	13.568	80.557	70.391	14.232	-79.933	-50.965	7.956
1500	13.667	81.497	71.101	15.594	-79.887	-48.898	7.124
1600	13.759	82.382	71.778	16.966	-79.840	-46.833	6.397
1700	13.844	83.219	72.427	18.346	-79.795	-44.772	5.756
1800	13.921	84.012	73.049	19.734	-79.752	-42.712	5.186
1900	13.992	84.767	73.646	21.130	-79.710	-40.657	4.677
2000	14.057	85.486	74.220	22.532	-79.673	-38.601	4.218

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.299 + 0.908 \times 10^{-3}T - 0.609 \times 10^{5}T^{-2}$
$H° - H°_{298} = 12.299 \times 10^{-3}T + 0.454 \times 10^{-6}T^{2} + 0.609 \times 10^{2}T^{-1} - 3.912$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -62.167 + 2.320 \times 10^{-3}T - 7.654 \times 10^{-6}T^{2} + 46.550T^{-1}$
$\Delta Gf° = -62.167 - 2.320 \times 10^{-3}T\ln T + 7.654 \times 10^{-6}T^{2} + 23.275T^{-1} + 10.846 \times 10^{-3}T$
301.55-952 K: $\Delta Hf° = -62.311 - 1.677 \times 10^{-3}T - 0.122 \times 10^{-6}T^{2} + 95.850T^{-1}$
$\Delta Gf° = -62.311 + 1.677 \times 10^{-3}T\ln T + 0.122 \times 10^{-6}T^{2} + 47.925T^{-1} - 9.498 \times 10^{-3}T$
952-2000 K: $\Delta Hf° = -80.846 + 0.697 \times 10^{-3}T - 0.071 \times 10^{-6}T^{2} + 125.450T^{-1}$
$\Delta Gf° = -80.846 - 0.697 \times 10^{-3}T\ln T + 0.071 \times 10^{-6}T^{2} + 62.725T^{-1} + 26.287 \times 10^{-3}T$

Source: Data from Chase (81) who estimated some molecular constants.

$(CsOH)_2(g)$
Dimeric Cesium Hydroxide (ideal gas)
[Formation: $2Cs(c,l,g) + H_2(g) + O_2(g) = (CsOH)_2(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.791	86.195	86.195	0	-164.400	-154.037	112.911
300	19.818	86.317	86.195	.037	-164.417	-153.972	112.167
301.55	19.840	86.419	86.195	.068	-164.432	-153.918	111.551
301.55	19.840	86.419	86.195	.068	-165.432	-153.918	111.551
400	21.264	92.217	86.990	2.091	-166.291	-150.029	81.971
500	22.577	97.107	88.537	4.285	-167.025	-145.876	63.762
600	23.665	101.323	90.325	6.599	-167.650	-141.585	51.572
700	24.552	105.040	92.167	9.011	-168.198	-137.196	42.834
800	25.289	108.368	93.988	11.504	-168.689	-132.736	36.261
900	25.918	111.384	95.756	14.065	-169.131	-128.214	31.134
952	26.203	112.849	96.650	15.421	-169.346	-125.869	28.895
952	26.203	112.849	96.650	15.421	-201.742	-125.869	28.895
1000	26.467	114.144	97.459	16.685	-201.698	-122.044	26.672
1100	26.952	116.689	99.092	19.357	-201.585	-114.081	22.666
1200	27.384	119.053	100.658	22.074	-201.444	-106.130	19.329
1300	27.770	121.261	102.159	24.832	-201.282	-98.195	16.508
1400	28.116	123.332	103.598	27.627	-201.103	-90.272	14.092
1500	28.427	125.282	104.979	30.454	-200.907	-82.362	12.000
1600	28.704	127.126	106.307	33.311	-200.702	-74.467	10.172
1700	28.954	128.874	107.583	36.194	-200.488	-66.582	8.560
1800	29.178	130.535	108.812	39.101	-200.270	-58.711	7.128
1900	29.379	132.118	109.997	42.029	-200.050	-50.854	5.850
2000	29.560	133.630	111.142	44.976	-199.833	-43.007	4.700

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.597 + 4.738\times10^{-3}T - 2.861\times10^{5}T^{-2}$
$H° - H°_{298} = 21.597\times10^{-3}T + 2.369\times10^{-6}T^{2} + 2.861\times10^{2}T^{-1} - 7.609$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -164.521 + 1.639\times10^{-3}T - 13.847\times10^{-6}T^{2} + 257.400T^{-1}$
$\Delta Gf° = -164.521 - 1.639\times10^{-3}T\ln T + 13.847\times10^{-6}T^{2} + 128.700T^{-1} + 38.925\times10^{-3}T$
301.55-952 K: $\Delta Hf° = -164.807 - 6.355\times10^{-3}T + 1.217\times10^{-6}T^{2} + 356.000T^{-1}$
$\Delta Gf° = -164.807 + 6.355\times10^{-3}T\ln T - 1.217\times10^{-6}T^{2} + 178.000T^{-1} - 1.763\times10^{-3}T$
952-2000 K: $\Delta Hf° = -201.878 - 1.607\times10^{-3}T + 1.319\times10^{-6}T^{2} + 415.200T^{-1}$
$\Delta Gf° = -201.878 + 1.607\times10^{-3}T\ln T - 1.319\times10^{-6}T^{2} + 207.600T^{-1} + 69.806\times10^{-3}T$

Source: Data from Chase (81) who estimated molecular constants.

$CsPO_3(c)$
Cesium Metaphosphate

[Formation: $Cs(c,l) + P(c,l,1/4P_4(g)) + 1.5O_2(g) = CsPO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	24.280	30.430	30.430	0	-296.700	-274.855	201.472
300	24.310	30.580	30.447	.040	-296.704	-274.725	200.134
301.55	24.334	30.705	30.448	.078	-296.704	-274.611	199.023
301.55	24.334	30.705	30.448	.078	-297.204	-274.611	199.023
317.3	24.575	31.950	30.492	.463	-297.197	-273.430	188.331
317.3	24.575	31.950	30.492	.463	-297.354	-273.430	188.331
400	25.840	37.780	31.405	2.550	-297.298	-267.196	145.987
500	27.370	43.710	33.290	5.210	-297.112	-259.689	113.509
550	28.135	46.359	34.351	6.604	-296.966	-255.963	101.709
550	28.135	46.359	34.351	6.604	-299.874	-255.963	101.709
600	28.900	48.840	35.457	8.030	-299.623	-251.982	91.783
700	30.430	53.410	37.710	10.990	-299.042	-244.092	76.208
800	31.960	57.570	39.932	14.110	-298.337	-236.289	64.550

*Data except enthalpy of formation at 298 K estimated.

Phase changes:
301.55 K, melting point of Cs; $\Delta H^\circ = 0.500$ kcal/mol.
317.3 K, melting point of P; $\Delta H^\circ = 0.157$ kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H^\circ = 2.908$ kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K:
$Cp^\circ = 19.720 + 15.300\text{x}10^{-3}T$
$H^\circ - H^\circ_{298} = 19.720\text{x}10^{-3}T + 7.650\text{x}10^{-6}T^2 - 6.560$

Formation equations (kcal/mol):

298.15-301.55 K:
$\Delta Hf^\circ = -296.701 + 1.940\text{x}10^{-3}T - 3.937\text{x}10^{-6}T^2 - 67.800T^{-1}$
$\Delta Gf^\circ = -296.701 - 1.940\text{x}10^{-3}T\ln T + 3.937\text{x}10^{-6}T^2 - 33.900T^{-1} + 83.532\text{x}10^{-3}T$

301.55-317.3 K:
$\Delta Hf^\circ = -296.844 - 2.057\text{x}10^{-3}T + 3.595\text{x}10^{-6}T^2 - 18.500T^{-1}$
$\Delta Gf^\circ = -296.844 + 2.057\text{x}10^{-3}T\ln T - 3.595\text{x}10^{-6}T^2 - 9.250T^{-1} + 63.188\text{x}10^{-3}T$

317.3-550 K:
$\Delta Hf^\circ = -296.531 - 4.550\text{x}10^{-3}T + 6.780\text{x}10^{-6}T^2 - 18.500T^{-1}$
$\Delta Gf^\circ = -296.531 + 4.550\text{x}10^{-3}T\ln T - 6.780\text{x}10^{-6}T^2 - 9.250T^{-1} + 48.852\text{x}10^{-3}T$

550-800 K:
$\Delta Hf^\circ = -299.991 - 3.212\text{x}10^{-3}T + 6.776\text{x}10^{-6}T^2 - 118.800T^{-1}$
$\Delta Gf^\circ = -299.991 + 3.212\text{x}10^{-3}T\ln T - 6.776\text{x}10^{-6}T^2 - 59.400T^{-1} + 63.750\text{x}10^{-3}T$

Sources: Enthalpy of formation from Wagman (516). Other data are those estimated by Beglov (25).

Cs_2SO_4(c,l)
Cesium Sulfate
[Reaction: $2Cs(c,l,g) + 0.5S_2(g) + 2O_2(g) = Cs_2SO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	32.619	50.640	50.640	0	-360.325	-325.930	238.910
300	32.697	50.842	50.642	.060	-360.326	-325.715	237.280
301.55	32.750	51.011	50.643	.111	-360.327	-325.536	235.931
301.55	32.750	51.011	50.643	.111	-361.327	-325.536	235.931
400	36.090	60.741	51.969	3.509	-361.220	-313.861	171.483
500	39.097	69.114	54.580	7.267	-360.836	-302.060	132.029
600	42.455	76.532	57.630	11.341	-360.180	-290.360	105.762
700	46.388	83.363	60.823	15.778	-359.209	-278.794	87.042
800	50.959	89.849	64.049	20.640	-357.859	-267.397	73.049
900	56.175	96.146	67.267	25.991	-356.053	-256.192	62.211
952	59.208	99.380	68.932	28.987	-354.915	-250.478	57.501
952	59.208	99.380	68.932	28.987	-387.311	-250.478	57.501
997	61.832	102.175	70.370	31.710	-385.981	-244.041	53.495
997	46.293	102.248	70.370	31.782	-385.909	-244.041	53.495
1000	46.405	102.387	70.466	31.921	-385.863	-243.613	53.241
1100	50.109	106.984	73.578	36.747	-384.156	-229.467	45.590
1200	53.813	111.502	76.549	41.943	-382.100	-215.490	39.246
1278	56.702	114.981	78.790	46.253	-380.253	-204.718	35.008
1278	49.393	121.609	78.790	54.723	-371.783	-204.718	35.008
1300	49.393	122.452	79.522	55.809	-371.394	-201.847	33.933
1400	49.393	126.112	82.720	60.749	-369.637	-188.870	29.484
1500	49.393	129.520	85.728	65.688	-367.894	-176.020	25.646
1600	49.393	132.708	88.566	70.627	-366.172	-163.286	22.303
1700	49.393	135.702	91.251	75.567	-364.466	-150.656	19.368
1800	49.393	138.526	93.800	80.506	-362.779	-138.127	16.771
1900	49.393	141.196	96.225	85.445	-361.111	-125.694	14.458
2000	49.393	143.730	98.537	90.385	-359.464	-113.345	12.386

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.
997 K, transition point of Cs_2SO_4; ΔH° = 0.072 kcal/mol.
1278 K, melting point of Cs_2SO_4; ΔH° = 8.470 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-997 K: $Cp^\circ = 15.285 + 44.602\times10^{-3}T + 3.585\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 15.285\times10^{-3}T + 22.301\times10^{-6}T^{2} - 3.585\times10^{2}T^{-1} - 5.337$
997-1278 K: $Cp^\circ = 4.211 + 40.192\times10^{-3}T + 19.976\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 4.211\times10^{-3}T + 20.096\times10^{-6}T^{2} - 19.976\times10^{2}T^{-1} + 9.612$
1278-2000 K: $Cp^\circ = 49.393$
$H^\circ - H^\circ_{298} = 49.393\times10^{-3}T - 8.401$

Reaction equations (kcal/mol):

298.15-301.55 K: $\Delta Hr^\circ = -356.356 - 9.619\times10^{-3}T + 5.841\times10^{-6}T^{2} - 483.050T^{-1}$
$\Delta Gr^\circ = -356.356 + 9.619\times10^{-3}T\ln T - 5.841\times10^{-6}T^{2} - 241.525T^{-1} + 51.708\times10^{-3}T$
301.55-952 K: $\Delta Hr^\circ = -356.643 - 17.613\times10^{-3}T + 20.905\times10^{-6}T^{2} - 384.450T^{-1}$
$\Delta Gr^\circ = -356.643 + 17.613\times10^{-3}T\ln T - 20.905\times10^{-6}T^{2} - 192.225T^{-1} + 11.021\times10^{-3}T$
952-997 K: $\Delta Hr^\circ = -393.713 - 12.865\times10^{-3}T + 21.007\times10^{-6}T^{2} - 325.250T^{-1}$
$\Delta Gr^\circ = -393.713 + 12.865\times10^{-3}T\ln T - 21.007\times10^{-6}T^{2} - 162.625T^{-1} + 82.589\times10^{-3}T$
997-1278 K: $\Delta Hr^\circ = -378.765 - 23.939\times10^{-3}T + 18.802\times10^{-6}T^{2} - 1964.350T^{-1}$
$\Delta Gr^\circ = -378.765 + 23.939\times10^{-3}T\ln T - 18.802\times10^{-6}T^{2} - 982.175T^{-1} - 10.241\times10^{-3}T$
1278-2000 K: $\Delta Hr^\circ = -396.778 + 21.244\times10^{-3}T - 1.294\times10^{-6}T^{2} + 33.250T^{-1}$
$\Delta Gr^\circ = -396.778 - 21.244\times10^{-3}T\ln T + 1.294\times10^{-6}T^{2} + 16.625T^{-1} + 300.748\times10^{-3}T$

Source: Data from DeKock (113).

$Cs_2SO_4(g)$
Cesium Sulfate (ideal gas)
[Reaction: $2Cs(c,l,g) + 0.5S_2(g) + 2O_2(g) = Cs_2SO_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	26.307	97.126	97.126	0	-283.655	-263.119	192.869
300	26.373	97.289	97.126	.049	-283.667	-262.990	191.586
301.55	26.420	97.425	97.127	.090	-283.678	-262.883	190.524
301.55	26.420	97.425	97.127	.090	-284.678	-262.883	190.524
400	29.410	105.316	98.201	2.846	-285.213	-255.684	139.697
500	31.546	112.123	100.321	5.901	-285.531	-248.260	108.513
600	33.029	118.013	102.790	9.134	-285.716	-240.785	87.705
700	34.071	123.188	105.342	12.492	-285.825	-233.288	72.835
800	34.818	127.789	107.867	15.938	-285.891	-225.781	61.680
900	35.368	131.923	110.313	19.449	-285.925	-218.263	53.001
952	35.583	133.917	111.549	21.294	-285.937	-214.378	49.214
952	35.583	133.917	111.549	21.294	-318.333	-214.378	49.214
1000	35.781	135.672	112.665	23.007	-318.107	-209.142	45.707
1100	36.098	139.098	114.914	26.602	-317.632	-198.267	39.392
1200	36.346	142.250	117.063	30.225	-317.147	-187.435	34.136
1300	36.543	145.167	119.114	33.869	-316.664	-176.646	29.697
1400	36.702	147.881	121.072	37.532	-316.184	-165.893	25.897
1500	36.833	150.418	122.945	41.209	-315.702	-155.176	22.609
1600	36.940	152.799	124.738	44.898	-315.231	-144.490	19.736
1700	37.031	155.041	126.455	48.597	-314.766	-133.832	17.205
1800	37.107	157.160	128.103	52.303	-314.311	-123.201	14.958
1900	37.172	159.168	129.685	56.017	-313.869	-112.599	12.952
2000	37.227	161.076	131.208	59.737	-313.441	-102.016	11.148

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 33.664 + 2.338\times10^{-3}T - 7.160\times10^{5}T^{-2}$
$H°-H°_{298} = 33.664\times10^{-3}T + 1.169\times10^{-6}T^{2} + 7.160\times10^{2}T^{-1} - 12.542$

Reaction equations (kcal/mol):

298.15-301.55 K: $\Delta Hr° = -286.891 + 8.761\times10^{-3}T - 15.291\times10^{-6}T^{2} + 591.450T^{-1}$
$\Delta Gr° = -286.891 - 8.761\times10^{-3}T\ln T + 15.291\times10^{-6}T^{2} + 295.725T^{-1} + 121.760\times10^{-3}T$
301.55-952 K: $\Delta Hr° = -287.178 + 0.767\times10^{-3}T - 0.227\times10^{-6}T^{2} + 690.050T^{-1}$
$\Delta Gr° = -287.178 - 0.767\times10^{-3}T\ln T + 0.227\times10^{-6}T^{2} + 345.025T^{-1} + 81.072\times10^{-3}T$
952-2000 K: $\Delta Hr° = -324.248 + 5.515\times10^{-3}T - 0.125\times10^{-6}T^{2} + 749.250T^{-1}$
$\Delta Gr° = -324.248 - 5.515\times10^{-3}T\ln T + 0.125\times10^{-6}T^{2} + 374.625T^{-1} + 152.641\times10^{-3}T$

Source: Data from JANAF (130) who estimated some molecular constants.

$Cs_2UO_4(c)$
Cesium Uranate
[Formation: $2Cs(c,l,g) + U(c) + 2O_2(g) = Cs_2UO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	36.510	52.500	52.500	0	-453.460	-424.167	310.919
300	36.569	52.726	52.500	.068	-453.458	-423.983	308.868
301.55	36.603	52.915	52.501	.125	-453.457	-423.831	307.170
301.55	36.603	52.915	52.501	.125	-454.457	-423.831	307.170
400	38.757	63.585	53.965	3.848	-454.308	-413.852	226.115
500	39.979	72.375	56.797	7.789	-454.063	-403.765	176.483
600	40.831	79.743	60.025	11.831	-453.812	-393.729	143.414
700	41.507	86.090	63.306	15.949	-453.598	-383.732	119.805
800	42.089	91.671	66.508	20.130	-453.446	-373.766	102.107
900	42.617	96.659	69.587	24.365	-453.366	-363.810	88.344
942	42.825	98.608	70.838	26.159	-453.359	-359.655	83.441
942	42.825	98.608	70.838	26.159	-454.026	-359.655	83.441
952	42.874	99.060	71.131	26.588	-454.012	-358.654	82.335
952	42.874	99.060	71.131	26.588	-486.408	-358.654	82.335
1000	43.112	101.175	72.523	28.652	-486.110	-352.219	76.976
1049	43.343	103.243	73.910	30.770	-485.800	-345.665	72.015
1049	43.343	103.243	73.910	30.770	-486.937	-345.665	72.015
1100	43.584	105.306	75.318	32.987	-486.553	-338.804	67.313

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 39.377 + 4.096\times10^{-3}T - 3.614\times10^{5}T^{-2}$
$H°- H°_{298} = 39.377\times10^{-3}T + 2.048\times10^{-6}T^{2} + 3.614\times10^{2}T^{-1} - 13.134$

Formation equations (kcal/mol):

298.15-301.55 K: $ΔHf° = -457.652 + 15.535\times10^{-3}T - 18.474\times10^{-6}T^{2} + 358.500T^{-1}$
$ΔGf° = -457.652 - 15.535\times10^{-3}T\ln T + 18.474\times10^{-6}T^{2} + 179.250T^{-1} + 193.298\times10^{-3}T$

301.55-942 K: $ΔHf° = -457.938 + 7.541\times10^{-3}T - 3.410\times10^{-6}T^{2} + 457.100T^{-1}$
$ΔGf° = -457.938 - 7.541\times10^{-3}T\ln T + 3.410\times10^{-6}T^{2} + 228.550T^{-1} + 152.610\times10^{-3}T$

942-952 K: $ΔHf° = -455.528 + 0.396\times10^{-3}T + 0.812\times10^{-6}T^{2} + 369.600T^{-1}$
$ΔGf° = -455.528 - 0.396\times10^{-3}T\ln T - 0.812\times10^{-6}T^{2} + 184.800T^{-1} + 105.149\times10^{-3}T$

952-1049 K: $ΔHf° = -492.599 + 5.144\times10^{-3}T + 0.914\times10^{-6}T^{2} + 428.800T^{-1}$
$ΔGf° = -492.599 - 5.144\times10^{-3}T\ln T - 0.914\times10^{-6}T^{2} + 214.400T^{-1} + 176.718\times10^{-3}T$

1049-1100 K: $ΔHf° = -494.895 + 6.249\times10^{-3}T + 0.914\times10^{-6}T^{2} + 428.800T^{-1}$
$ΔGf° = -494.895 - 6.249\times10^{-3}T\ln T - 0.914\times10^{-6}T^{2} + 214.400T^{-1} + 186.592\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from O'Hare (369). Low-temperature heat capacities and entropy at 298 K from Osborne (377). High-temperature data based on Fredrickson (160).

$Cs_2U_4O_{12}$(c)
Cesium Tetrauranate
[Formation: $2Cs(c,l,g) + 4U(c) + 6O_2(g) = Cs_2U_4O_{12}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^{o}_{298})/T$	$H°- H^{o}_{298}$	ΔHf°	ΔGf°	
298.15	91.780	125.820	125.820	0	-1332.200	-1255.590	920.361
300	91.990	126.390	125.823	.170	-1332.184	-1255.113	914.337
301.55	92.115	126.864	125.827	.313	-1332.172	-1254.715	909.349
301.55	92.115	126.864	125.827	.313	-1333.172	-1254.715	909.349
400	100.030	154.080	129.530	9.820	-1332.062	-1229.249	671.622
500	104.670	176.940	136.800	20.070	-1330.640	-1203.708	526.134
600	107.980	196.330	145.147	30.710	-1329.202	-1178.457	429.247
700	110.660	213.180	153.694	41.640	-1327.892	-1153.438	360.115
800	113.000	228.110	162.073	52.830	-1326.782	-1128.600	308.315
898	115.100	241.290	170.010	64.010	-1325.944	-1104.368	268.771
898	124.130	242.170	170.010	64.800	-1325.154	-1104.368	268.771
900	124.230	242.450	170.172	65.050	-1325.120	-1103.878	268.055
942	126.491	248.167	173.525	70.313	-1324.447	-1093.598	253.718
942	126.491	248.167	173.525	70.313	-1327.115	-1093.598	253.718
952	127.029	249.506	174.316	71.581	-1326.900	-1091.121	250.484
952	127.029	249.506	174.316	71.581	-1359.296	-1091.121	250.484
968	127.890	251.630	175.576	73.620	-1358.868	-1086.617	245.327

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
898 K, transition point of $Cs_2U_4O_{12}$; ΔH° = 0.790 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-898 K: $Cp° = 101.322 + 17.144x10^{-3}T - 13.026x10^{5}T^{-2}$
$H°- H^{o}_{298} = 101.322x10^{-3}T + 8.572x10^{-6}T^{2} + 13.026x10^{2}T^{-1} - 35.340$
898-968 K: $Cp° = 75.913 + 53.690x10^{-3}T$
$H°- H^{o}_{298} = 75.913x10^{-3}T + 26.845x10^{-6}T^{2} - 25.018$

Formation equations (kcal/mol):

298.15-301.55 K: $ΔHf° = -1346.162 + 39.230x10^{-3}T - 26.628x10^{-6}T^{2} + 1381.400T^{-1}$
$ΔGf° = -1346.162 - 39.230x10^{-3}TlnT + 26.628x10^{-6}T^{2} + 690.700T-1+ 511.588x10^{-3}T$
301.55-898 K: $ΔHf° = -1346.449 + 31.236x10^{-3}T - 11.564x10^{-6}T^{2} + 1480\ T^{-1}$
$ΔGf° = -1346.449 - 31.236x10^{-3}TlnT + 11.564x10^{-6}T^{2} + 740\ T-1+ 470.900x10^{-3}T$
898-942 K: $ΔHf° = -1336.126 + 5.827x10^{-3}T + 6.709x10^{-6}T^{2} + 177.400T^{-1}$
$ΔGf° = -1336.126 - 5.827x10^{-3}TlnT - 6.709x10^{-6}T^{2} + 88.700T-1+ 303.836x10^{-3}T$
942-952 K: $ΔHf° = -1326.486 - 22.753x10^{-3}T + 23.597x10^{-6}T^{2} - 172.600T^{-1}$
$ΔGf° = -1326.486 + 22.753x10^{-3}TlnT - 23.597x10^{-6}T^{2} - 86.300T-1+ 113.992x10^{-3}T$
952-968 K: $ΔHf° = -1363.557 - 18.005x10^{-3}T + 23.699x10^{-6}T^{2} - 113.400T^{-1}$
$ΔGf° = -1363.557 + 18.005x10^{-3}TlnT - 23.699x10^{-6}T^{2} - 56.700T-1+ 185.561x10^{-3}T$

Source: Data from Cordfunke (100).

$CuCN(c)$
Copper Cyanide
[Formation: $Cu(c) + C(c) + 0.5N_2(g) = CuCN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	14.585	21.511	21.511	0	22.700	25.881	-18.971
300	14.620	21.601	21.511	.027	22.706	25.901	-18.869
350	15.450	23.938	21.695	.785	22.882	26.420	-16.497
400	15.950	26.035	22.108	1.571	23.063	26.913	-14.705
450	16.390	27.940	22.653	2.379	23.241	27.382	-13.298

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-450 K: $Cp^\circ = 23.790 - 11.460\times10^{-3}T - 5.140\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 23.790\times10^{-3}T - 5.730\times10^{-6}T^2 + 5.140\times10^{2}T^{-1} - 8.308$

Formation equations (kcal/mol):

298.15-450 K: $\Delta Hf^\circ = 18.706 + 11.693\times10^{-3}T - 7.601\times10^{-6}T^2 + 352.650T^{-1}$

$\Delta Gf^\circ = 18.706 - 11.693\times10^{-3}T\ln T + 7.601\times10^{-6}T^2 + 176.325T^{-1} + 86.440\times10^{-3}T$

Source: Data from King (267).

$CuCr_2O_4(c)$
Copper Chromate
[Formation: $Cu(c) + 2Cr(c) + 2O_2(g) = CuCr_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	31.800	36.000	36.000	0	-315.300	-291.080	213.365
300	31.900	36.200	36.000	.060	-315.297	-290.931	211.941
311.5	32.279	37.407	36.030	.429	-315.291	-289.997	203.461
400	35.200	45.830	37.305	3.410	-315.123	-282.835	154.532
500	38.000	54.000	39.840	7.080	-314.771	-274.794	120.111
600	40.000	61.110	42.810	10.980	-314.323	-266.840	97.195
700	41.500	67.390	45.876	15.060	-313.812	-258.959	80.850
800	42.500	73.000	48.925	19.260	-313.283	-251.165	68.614
888	59.800	77.910	51.551	23.407	-312.432	-244.369	60.142
900	53.000	78.670	51.903	24.090	-312.204	-243.447	59.116
1000	44.000	83.370	54.830	28.540	-311.588	-235.857	51.546
1100	44.300	87.580	57.616	32.960	-311.110	-228.301	45.359

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
880 K, second order transition point of $CuCr_2O_4$; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-888 K: $Cp° = 27.647 + 21.588x10^{-3}T - 2.031x10^{5}T^{-2}$
$H°- H°_{298} = 27.647x10^{-3}T + 10.794x10^{-6}T^{2} + 2.031x10^{2}T^{-1} - 9.884$
888-1100 K: $Cp° = 57.434 - 13.428x10^{-3}T + 9.533x10^{5}T^{-2}$
$H°- H°_{298} = 57.434x10^{-3}T - 6.714x10^{-6}T^{2} - 9.533x10^{2}T^{-1} - 21.227$

Formation equations (kcal/mol):

298.15-311.5 K: $ΔHf° = -318.019 + 13.483x10^{-3}T - 19.156x10^{-6}T^{2} + 119.700T^{-1}$
$ΔGf° = -318.019 - 13.483x10^{-3}TlnT + 19.156x10^{-6}T^{2} + 59.850T^{-1} + 160.788x10^{-3}T$
311.5-888 K: $ΔHf° = -316.023 - 0.851x10^{-3}T + 5.396x10^{-6}T^{2} + 146.900T^{-1}$
$ΔGf° = -316.023 + 0.851x10^{-3}TlnT - 5.396x10^{-6}T^{2} + 73.450T^{-1} + 79.593x10^{-3}T$
888-1100 K: $ΔHf° = -327.366 + 28.936x10^{-3}T - 12.112x10^{-6}T^{2} - 1009.500T^{-1}$
$ΔGf° = -327.366 - 28.936x10^{-3}TlnT + 12.112x10^{-6}T^{2} - 504.750T^{-1} + 279.776x10^{-3}T$

Sources: Enthalpy of formation at 298 K from King (267). Entropy at 298 K based on Rog (429). Other data from Reznitskii (420).

$CuFeO_2(c,l)$
Cuprous Ferrite
[Formation: $Cu(c,l) + Fe(c) + O_2(g) = CuFeO_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	19.131	21.241	21.241	0	-122.500	-109.916	80.569
300	19.179	21.359	21.242	.035	-122.500	-109.838	80.016
400	21.278	27.192	22.022	2.068	-122.397	-105.629	57.712
500	22.597	32.093	23.559	4.267	-122.223	-101.456	44.346
600	23.410	36.291	25.341	6.570	-122.038	-97.320	35.448
700	23.908	39.940	27.171	8.938	-121.882	-93.213	29.102
800	24.239	43.155	28.972	11.346	-121.788	-89.126	24.348
900	24.514	46.026	30.710	13.784	-121.789	-85.044	20.651
1000	24.800	48.624	32.374	16.250	-121.962	-80.955	17.692
1043	24.940	49.671	33.066	17.319	-122.181	-79.188	16.593
1091	25.096	50.796	33.821	18.520	-122.309	-77.203	15.465
1091	25.802	50.879	33.821	18.610	-122.219	-77.203	15.465
1100	25.834	51.091	33.961	18.843	-122.232	-76.832	15.265
1185	26.143	53.026	35.261	21.051	-122.234	-73.325	13.523
1185	26.143	53.026	35.261	21.051	-122.449	-73.325	13.523
1200	26.197	53.355	35.485	21.444	-122.415	-72.704	13.241
1300	26.559	55.466	36.941	24.082	-122.199	-68.570	11.528
1357.6	26.768	56.621	37.752	25.618	-122.092	-66.198	10.657
1357.6	26.768	56.621	37.752	25.618	-125.212	-66.198	10.657
1400	26.922	57.447	38.336	26.756	-125.131	-64.357	10.046
1470	27.176	58.767	39.277	28.650	-124.992	-61.322	9.117
1470	30.284	69.230	39.277	44.030	-109.612	-61.322	9.117
1500	30.284	69.842	39.883	44.938	-109.460	-60.340	8.791
1600	30.284	71.796	41.817	47.967	-108.969	-57.078	7.796

Phase changes:
1043 K, Curie temperature of Fe; $\Delta H° = 0$ kcal/mol.
1091 K, $\alpha - \beta$ transition point of $CuFeO_2$; $\Delta H° = 0.090$ kcal/mol.
1185 K, $\alpha - \gamma$ transition point of Fe; $\Delta H° = 0.215$ kcal/mol.
1357.6 K, melting point of Cu; $\Delta H° = 3.120$ kcal/mol.
1470 K, melting point of $CuFeO_2$; $\Delta H° = 15.380$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1091 K: $Cp° = 22.910 + 2.420\times10^{-3}T - 4.010\times10^{5}T^{-2}$
$H°-H°_{298} = 22.910\times10^{-3}T + 1.210\times10^{-6}T^2 + 4.010\times10^{2}T^{-1} - 8.283$
1091-1470 K: $Cp° = 21.824 + 3.642\times10^{-3}T + 0.061\times10^{5}T^{-2}$
$H°-H°_{298} = 21.824\times10^{-3}T + 1.821\times10^{-6}T^2 - 0.061\times10^{2}T^{-1} - 7.362$
1470-1600 K: $Cp° = 30.284$
$H°-H°_{298} = 30.284\times10^{-3}T - 0.487$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf° = -127.089 + 10.581\times10^{-3}T - 6.174\times10^{-6}T^2 + 591.300T^{-1}$
$\Delta Gf° = -127.089 - 10.581\times10^{-3}T\ln T + 6.174\times10^{-6}T^2 + 295.650T^{-1} + 112.720\times10^{-3}T$
1043-1091 K: $\Delta Hf° = -103.528 - 33.400\times10^{-3}T + 14.537\times10^{-6}T^2 + 362.800T^{-1}$
$\Delta Gf° = -103.528 + 33.400\times10^{-3}T\ln T - 14.537\times10^{-6}T^2 + 181.400T^{-1} - 193.825\times10^{-3}T$
1091-1185 K: $\Delta Hf° = -102.608 - 34.486\times10^{-3}T + 15.148\times10^{-6}T^2 - 44.300T^{-1}$
$\Delta Gf° = -102.608 + 34.486\times10^{-3}T\ln T - 15.148\times10^{-6}T^2 - 22.150T^{-1} - 201.428\times10^{-3}T$
1185-1357.6 K: $\Delta Hf° = -126.222 + 3.769\times10^{-3}T - 0.543\times10^{-6}T^2 + 74.700T^{-1}$
$\Delta Gf° = -126.222 - 3.769\times10^{-3}T\ln T + 0.543\times10^{-6}T^2 + 37.350T^{-1} + 70.613\times10^{-3}T$
1357.6-1470 K: $\Delta Hf° = -127.462 + 1.289\times10^{-3}T + 0.267\times10^{-6}T^2 + 67.700T^{-1}$
$\Delta Gf° = -127.462 - 1.289\times10^{-3}T\ln T - 0.267\times10^{-6}T^2 + 33.850T^{-1} + 54.739\times10^{-3}T$
1470-1600 K: $\Delta Hf° = -120.588 + 9.749\times10^{-3}T - 1.554\times10^{-6}T^2 + 73.800T^{-1}$
$\Delta Gf° = -120.588 - 9.749\times10^{-3}T\ln T + 1.554\times10^{-6}T^2 + 36.900T^{-1} + 109.083\times10^{-3}T$

Source: Data from King (267).

$CuFe_2O_4(c)$
Copper Ferrite
[Formation: $Cu(c,l) + 2Fe(c) + 2O_2(g) = CuFe_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	35.520	35.076	35.076	0	-231.000	-205.986	150.990
300	35.603	35.296	35.076	.066	-230.993	-205.830	149.945
400	41.136	46.339	36.544	3.918	-230.407	-197.520	107.918
500	45.320	55.988	39.490	8.249	-229.514	-189.398	82.785
600	48.708	64.558	42.966	12.955	-228.418	-181.473	66.101
675	51.040	70.436	45.695	16.700	-227.495	-175.658	56.873
675	54.441	70.703	45.695	16.880	-227.315	-175.658	56.873
700	54.360	72.675	46.624	18.236	-226.922	-173.751	54.247
795	54.050	79.579	50.158	23.390	-225.541	-166.631	45.807
800	47.585	79.872	50.343	23.623	-225.512	-166.261	45.420
900	48.517	85.530	53.943	28.428	-224.922	-158.890	38.583
1000	49.469	90.691	57.364	33.327	-224.625	-151.575	33.126
1043	49.887	92.783	58.781	35.463	-224.771	-148.432	31.102
1100	50.441	95.452	60.613	38.323	-224.663	-144.258	28.661
1185	51.285	99.237	63.249	42.646	-224.155	-138.064	25.463
1185	51.285	99.237	63.249	42.646	-224.585	-138.064	25.463
1200	51.434	99.883	63.703	43.416	-224.423	-136.972	24.946
1300	52.447	104.040	66.648	48.610	-223.327	-129.728	21.809
1357.6	53.043	106.326	68.282	51.649	-222.696	-125.597	20.219
1357.6	53.043	106.326	68.282	51.649	-225.816	-125.597	20.219
1400	53.481	107.964	69.459	53.907	-225.341	-122.475	19.119
1500	54.535	111.690	72.152	59.307	-224.183	-115.169	16.780

Phase change:
675 K, α - β transition point of $CuFe_2O_4$; ΔH° = 0.180 kcal/mol.
795 K, Curie temperature of $CuFe_2O_4$; ΔH° = 0 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-675 K: $Cp° = 33.054 + 28.662\times10^{-3}T - 5.402\times10^{5}T^{-2}$
$H° - H°_{298} = 33.054\times10^{-3}T + 14.331\times10^{-6}T^{2} + 5.402\times10^{2}T^{-1} - 12.941$
675-795 K: $Cp° = 57.480 - 4.400\times10^{-3}T + 0.010\times10^{5}T^{-2}$
$H° - H°_{298} = 57.480\times10^{-3}T - 2.200\times10^{-6}T^{2} - 0.010\times10^{2}T^{-1} - 20.915$
795-1500 K: $Cp° = 38.340 + 10.620\times10^{-3}T + 4.922\times10^{5}T^{-2}$
$H° - H°_{298} = 38.340\times10^{-3}T + 5.310\times10^{-6}T^{2} - 4.922\times10^{2}T^{-1} - 9.827$

Formation equations (kcal/mol):

298.15-675 K: $\Delta Hf° = -238.187 + 13.716\times10^{-3}T + 0.373\times10^{-6}T^{2} + 913.800T^{-1}$
$\Delta Gf° = -238.187 - 13.716\times10^{-3}T\ln T - 0.373\times10^{-6}T^{2} + 456.900T^{-1} + 181.125\times10^{-3}T$
675-795 K: $\Delta Hf° = -246.161 + 38.142\times10^{-3}T - 16.158\times10^{-6}T^{2} + 372.600T^{-1}$
$\Delta Gf° = -246.161 - 38.142\times10^{-3}T\ln T + 16.158\times10^{-6}T^{2} + 186.300T^{-1} + 341.501\times10^{-3}T$
795-1043 K: $\Delta Hf° = -235.074 + 19.002\times10^{-3}T - 8.648\times10^{-6}T^{2} - 118.600T^{-1}$
$\Delta Gf° = -235.074 - 19.002\times10^{-3}T\ln T + 8.648\times10^{-6}T^{2} - 59.300T^{-1} + 206.090\times10^{-3}T$
1043-1185 K: $\Delta Hf° = -187.952 - 68.960\times10^{-3}T + 32.774\times10^{-6}T^{2} - 575.600T^{-1}$
$\Delta Gf° = -187.952 + 68.960\times10^{-3}T\ln T - 32.774\times10^{-6}T^{2} - 287.800T^{-1} - 406.999\times10^{-3}T$
1185-1357.6 K: $\Delta Hf° = -235.180 + 7.550\times10^{-3}T + 1.392\times10^{-6}T^{2} - 337.600T^{-1}$
$\Delta Gf° = -235.180 - 7.550\times10^{-3}T\ln T - 1.392\times10^{-6}T^{2} - 168.800T^{-1} + 137.083\times10^{-3}T$
1357.6-1500 K: $\Delta Hf° = -236.421 + 5.070\times10^{-3}T + 2.202\times10^{-6}T^{2} - 344.600T^{-1}$
$\Delta Gf° = -236.421 - 5.070\times10^{-3}T\ln T - 2.202\times10^{-6}T^{2} - 172.300T^{-1} + 121.209\times10^{-3}T$

Source: Data from King (267).

CuH(g)
Copper Hydride (ideal gas)
[Formation: Cu(c,l) + 0.5H_2(g) = CuH(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	6.990	46.931	46.931	0	73.330	66.352	-48.637
300	6.991	46.974	46.931	.013	73.326	66.309	-48.306
400	7.087	48.996	47.206	.716	73.088	64.006	-34.971
500	7.258	50.595	47.729	1.433	72.843	61.763	-26.996
600	7.466	51.936	48.321	2.169	72.603	59.570	-21.698
700	7.677	53.103	48.923	2.926	72.370	57.417	-17.926
800	7.872	54.141	49.511	3.704	72.144	55.296	-15.106
900	8.045	55.079	50.079	4.500	71.922	53.203	-12.919
1000	8.196	55.934	50.622	5.312	71.699	51.136	-11.176
1100	8.325	56.722	51.142	6.138	71.470	49.090	-9.753
1200	8.437	57.451	51.638	6.976	71.225	47.067	-8.572
1300	8.533	58.130	52.111	7.825	70.954	45.064	-7.576
1357.6	8.581	58.502	52.374	8.318	70.781	43.918	-7.070
1357.6	8.581	58.502	52.374	8.318	67.661	43.918	-7.070
1400	8.617	58.766	52.564	8.683	67.534	43.178	-6.740
1500	8.691	59.363	52.998	9.548	67.235	41.448	-6.039
1600	8.757	59.926	53.413	10.421	66.939	39.740	-5.428
1700	8.815	60.458	53.812	11.299	66.644	38.048	-4.891
1800	8.867	60.964	54.196	12.183	66.350	36.373	-4.416
1900	8.915	61.444	54.563	13.073	66.057	34.719	-3.994
2000	8.958	61.903	54.920	13.966	65.762	33.075	-3.614

Phase change: 1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.370 + 0.900\text{x}10^{-3}T - 1.090\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 7.370\text{x}10^{-3}T + 0.450\text{x}10^{-6}T^{2} + 1.090\text{x}10^{2}T^{-1} - 2.603$

Formation equations (kcal/mol):

298.15-1357.6 K: $\Delta Hf° = 73.315 - 1.178\text{x}10^{-3}T - 0.570\text{x}10^{-6}T^{2} + 124.250T^{-1}$

$\Delta Gf° = 73.315 + 1.178\text{x}10^{-3}T\ln T + 0.570\text{x}10^{-6}T^{2} + 62.125T^{-1} - 30.934\text{x}10^{-3}T$

1357.6-2000 K: $\Delta Hf° = 72.074 - 3.658\text{x}10^{-3}T + 0.240\text{x}10^{-6}T^{2} + 117.250T^{-1}$

$\Delta Gf° = 72.074 + 3.658\text{x}10^{-3}T\ln T - 0.240\text{x}10^{-6}T^{2} + 58.625T^{-1} - 46.808\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Kant (233). Other data from King (267).

CuD(g)
Copper Deuteride (ideal gas)
[Formation: $Cu(c,l) + 0.5D_2(g) = CuD(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.099	48.332	48.332	0	73.700	66.813	-48.975
300	7.103	48.376	48.333	.013	73.695	66.770	-48.642
400	7.358	50.452	48.612	.736	73.475	64.497	-35.239
500	7.645	52.125	49.153	1.486	73.263	62.275	-27.220
600	7.906	53.543	49.770	2.264	73.063	60.097	-21.890
700	8.123	54.778	50.399	3.065	72.869	57.951	-18.093
800	8.298	55.875	51.016	3.887	72.678	55.834	-15.253
900	8.440	56.860	51.611	4.724	72.484	53.740	-13.050
1000	8.555	57.756	52.182	5.574	72.284	51.667	-11.292
1100	8.649	58.576	52.727	6.434	72.070	49.616	-9.858
1200	8.729	59.332	53.246	7.303	71.837	47.586	-8.666
1300	8.796	60.033	53.741	8.179	71.571	45.574	-7.662
1357.6	8.829	60.415	54.016	8.687	71.400	44.424	-7.151
1357.6	8.829	60.415	54.016	8.687	68.280	44.424	-7.151
1400	8.854	60.687	54.214	9.062	68.153	43.680	-6.819
1500	8.905	61.300	54.667	9.950	67.854	41.942	-6.111
1600	8.950	61.876	55.099	10.843	67.557	40.226	-5.495
1700	8.990	62.420	55.514	11.740	67.257	38.525	-4.953
1800	9.027	62.935	55.912	12.641	66.958	36.844	-4.473
1900	9.061	63.424	56.295	13.545	66.657	35.179	-4.046
2000	9.092	63.889	56.662	14.453	66.357	33.532	-3.664

*Enthalpy of formation at 298 K estimated.

Phase change: 1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.160 + 0.540 \times 10^{-3}T - 1.660 \times 10^{5}T^{-2}$

$H°- H°_{298} = 8.160 \times 10^{-3}T + 0.270 \times 10^{-6}T^{2} + 1.660 \times 10^{2}T^{-1} - 3.014$

Formation equations (kcal/mol):

298.15-1357.6 K: $\Delta Hf° = 73.232 - 0.292 \times 10^{-3}T - 0.855 \times 10^{-6}T^{2} + 188.050T^{-1}$

$\Delta Gf° = 73.232 + 0.292 \times 10^{-3}T\ln T + 0.855 \times 10^{-6}T^{2} + 94.025T^{-1} - 24.505 \times 10^{-3}T$

1357.6-2000 K: $\Delta Hf° = 71.991 - 2.772 \times 10^{-3}T - 0.045 \times 10^{-6}T^{2} + 181.050T^{-1}$

$\Delta Gf° = 71.991 + 2.772 \times 10^{-3}T\ln T + 0.045 \times 10^{-6}T^{2} + 90.525T^{-1} - 40.379 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K estimated. Other data from King (267).

$Cu(OH)_2(c)$
Copper Dihydroxide
[Formation: $Cu(c) + O_2(g) + H_2(g) = Cu(OH)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	21.000	20.800	20.800	0	-105.900	-85.824	62.910
300*	21.030	20.930	20.800	.039	-105.898	-85.699	62.431
350	21.700	24.223	21.060	1.107	-105.823	-82.338	51.414
400	22.220	27.155	21.643	2.205	-105.730	-78.990	43.157
450	22.660	29.798	22.405	3.327	-105.624	-75.654	36.742
500	23.050	32.206	23.266	4.470	-105.507	-72.331	31.615
550	23.420	34.421	24.181	5.632	-105.380	-69.019	27.425
600	23.770	36.474	25.122	6.811	-105.247	-65.720	23.938
650	24.090	38.389	26.069	8.008	-105.105	-62.431	20.991
700	24.390	40.185	27.014	9.220	-104.957	-59.153	18.468

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 20.808 + 5.520x10^{-3}T - 1.293x10^{5}T^{-2}$

$H°- H°_{298} = 20.808x10^{-3}T + 2.760x10^{-6}T^{2} + 1.293x10^{2}T^{-1} - 6.883$

Formation equations (kcal/mol):

298.15-700 K: $ΔHf° = -106.890 + 1.802x10^{-3}T + 1.028x10^{-6}T^{2} + 107.600T^{-1}$

$ΔGf° = -106.890 - 1.802x10^{-3}T\ln T - 1.028x10^{-6}T^{2} + 53.800T^{-1} + 80.623x10^{-3}T$

Source: Data from King (267) ,who estimated all above 298 K.

$CuO \cdot CuSO_4(c)$
Copper Oxysulfate
[Reaction: $2Cu(c) + 0.5S_2(g) + 2.5O_2(g) = CuO \cdot CuSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	$Cp°$	$S°$	$-(G° - H°_{298})/T$	$H° - H°_{298}$	$\Delta Hr°$	$\Delta Gr°$	
298.15	33.450	40.358	40.358	0	-234.455	-197.110	144.484
300	33.570	40.565	40.358	.062	-234.455	-196.877	143.423
400	38.092	50.876	41.734	3.657	-234.222	-184.378	100.738
500	41.376	59.750	44.470	7.640	-233.704	-171.973	75.168
600	43.701	67.511	47.678	11.900	-233.007	-159.689	58.166
700	45.332	74.378	51.011	16.357	-232.204	-147.530	46.060
800	46.539	80.513	54.322	20.953	-231.340	-135.495	37.015
900	47.587	86.055	57.545	25.659	-230.435	-123.568	30.006
1000	48.744	91.127	60.653	30.474	-229.483	-111.745	24.421
1100	50.278	95.840	63.640	35.420	-228.466	-100.017	19.871
1200	52.455	100.303	66.511	40.551	-227.336	-88.387	16.097

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 38.451 + 11.490 \times 10^{-3}T - 7.491 \times 10^{5}T^{-2}$

$H° - H°_{298} = 38.451 \times 10^{-3}T + 5.745 \times 10^{-6}T^{2} + 7.491 \times 10^{2}T^{-1} - 14.487$

Reaction equations (kcal/mol):

298.15-1200 K: $\Delta Hr° = -238.421 + 5.564 \times 10^{-3}T + 2.707 \times 10^{-6}T^{2} + 615.950T^{-1}$

$\Delta Gr° = -238.421 - 5.564 \times 10^{-3}T\ln T - 2.707 \times 10^{-6}T^{2} + 307.975T^{-1} + 167.603 \times 10^{-3}T$

Source: Data from King (267).

$CuSO_4(c)$
Copper Sulfate
[Reaction: $Cu(c) + 0.5S_2(g) + 2O_2(g) = CuSO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hr°$	$\Delta Gr°$	
298.15	23.632	26.173	26.173	0	-199.655	-167.749	122.962
300	23.710	26.319	26.173	.044	-199.655	-167.550	122.058
400	27.580	33.718	27.155	2.625	-199.487	-156.866	85.706
500	30.290	40.180	29.128	5.526	-199.074	-146.254	63.927
600	32.300	45.889	31.456	8.660	-198.499	-135.741	49.443
700	33.890	50.991	33.888	11.972	-197.813	-125.334	39.131
800	35.270	55.609	36.320	15.431	-197.036	-115.034	31.426
900	36.530	59.836	38.700	19.022	-196.176	-104.834	25.457
1000	37.700	63.747	41.013	22.734	-195.238	-94.736	20.704
1100	38.730	67.390	43.246	26.558	-194.232	-84.731	16.834

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 26.427 + 12.136\times10^{-3}T - 5.701\times10^{5}T^{-2}$

$H°- H°_{298} = 26.427\times10^{-3}T + 6.068\times10^{-6}T^{2} + 5.701\times10^{2}T^{-1} - 10.331$

Reaction equations (kcal/mol):

298.15-1100 K: $\Delta Hr° = -202.275 + 2.476\times10^{-3}T + 4.092\times10^{-6}T^{2} + 452.550T^{-1}$

$\Delta Gr° = -202.275 - 2.476\times10^{-3}T\ln T - 4.092\times10^{-6}T^{2} + 226.275T^{-1} + 128.579\times10^{-3}T$

Source: Data from DeKock (112).

$Cu_2SO_4(c)$
Dicopper Sulfate
[Reaction: $2Cu(c) + 0.5S_2(g) + 2O_2(g) = Cu_2SO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	31.000	43.600	43.600	0	-194.955	-165.882	121.593
300	31.068	43.792	43.602	.057	-194.953	-165.701	120.712
400	34.613	53.222	44.862	3.344	-194.673	-155.986	85.225
500	37.872	61.301	47.361	6.970	-194.146	-146.371	63.978
600	40.846	68.473	50.291	10.909	-193.394	-136.881	49.858
700	43.535	74.975	53.361	15.130	-192.437	-127.535	39.818

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = 24.179 + 28.398\times10^{-3}T - 1.463\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 24.179\times10^{-3}T + 14.199\times10^{-6}T^{2} + 1.463\times10^{2}T^{-1} - 8.962$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta Hr^\circ = -194.571 - 5.092\times10^{-3}T + 11.413\times10^{-6}T^{2} + 35.750T^{-1}$
$\Delta Gr^\circ = -194.571 + 5.092\times10^{-3}T\ln T - 11.413\times10^{-6}T^{2} + 17.875T^{-1} + 70.410\times10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$CuSO_4 \cdot H_2O(c)$
Copper Sulfate Monohydrate
[Reaction: $Cu(c) + 0.5S_2(g) + 2.5O_2(g) + H_2(g) = CuSO_4 \cdot H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	$Cp°$	$S°$	$-(G° - H°_{298})/T$	$H° - H°_{298}$	$\Delta Hr°$	$\Delta Gr°$	
298.15	32.013	34.900	34.900	0	-274.875	-228.961	167.831
300*	32.180	35.099	34.902	.059	-274.879	-228.676	166.588
350	36.678	40.397	35.308	1.781	-274.877	-220.972	137.980
400	41.176	45.588	36.271	3.727	-274.673	-213.283	116.531
450	45.674	50.698	37.591	5.898	-274.268	-205.632	99.867
500	50.172	55.743	39.153	8.295	-273.658	-198.036	86.560
550	54.670	60.736	40.889	10.916	-272.845	-190.511	75.701

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 4.421 + 91.380 \times 10^{-3}T + 0.308 \times 10^{5}T^{-2}$

$H° - H°_{298} = 4.421 \times 10^{-3}T + 45.690 \times 10^{-6}T^{2} - 0.308 \times 10^{2}T^{-1} - 5.276$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -269.358 - 29.602 \times 10^{-3}T + 43.044 \times 10^{-6}T^{2} - 154.450T^{-1}$

$\Delta Gr° = -269.358 + 29.602 \times 10^{-3}T\ln T - 43.044 \times 10^{-6}T^{2} - 77.225T^{-1} - 19.464 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all above 298 K.

$CuSO_4 \cdot 3H_2O(c)$
Copper Sulfate Trihydrate
[Reaction: $Cu(c) + 0.5S_2(g) + 3.5O_2(g) + 3H_2(g) = CuSO_4 \cdot 3H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	49.000	52.900	52.900	0	-417.915	-344.148	252.264
300*	49.244	53.204	52.901	.091	-417.926	-343.690	250.375
350	55.843	61.290	53.524	2.718	-418.064	-331.302	206.872
400	62.443	69.178	54.991	5.675	-417.902	-318.915	174.245
450	69.042	76.914	56.998	8.962	-417.442	-306.567	148.887
500	75.641	84.530	59.372	12.579	-416.680	-294.285	128.630
550	82.240	92.048	62.001	16.526	-415.615	-282.094	112.092

*Data above 298 k estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 9.534 + 132.174 \times 10^{-3}T + 0.052 \times 10^{5}T^{-2}$

$H° - H°_{298} = 9.534 \times 10^{-3}T + 66.087 \times 10^{-6}T^{2} - 0.052 \times 10^{2}T^{-1} - 8.700$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -409.656 - 44.631 \times 10^{-3}T + 62.099 \times 10^{-6}T^{2} - 141.050T^{-1}$

$\Delta Gr° = -409.656 + 44.631 \times 10^{-3}T\ln T - 62.099 \times 10^{-6}T^{2} - 70.525T^{-1} - 15.265 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all above 298 K.

$CuSO_4 \cdot 5H_2O(c)$
Copper Sulfate Pentahydrate
[Reaction: $Cu(c) + 0.5S_2(g) + 4.5O_2(g) + 5H_2(g) = CuSO_4 \cdot 5H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	67.027	71.800	71.800	0	-560.225	-458.873	336.359
300*	67.360	72.216	71.803	.124	-560.242	-458.245	333.827
350	76.354	83.275	72.655	3.717	-560.459	-441.222	275.508
400	85.348	94.057	74.657	7.760	-560.264	-424.195	231.766
450	94.342	104.629	77.402	12.252	-559.661	-407.219	197.770
500	103.336	115.035	80.647	17.194	-558.641	-390.332	170.612
550	112.330	125.305	84.240	22.586	-557.205	-373.566	148.440

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 13.142 + 180.360x10^{-3}T + 0.098x10^{5}T^{-2}$
$H°- H°_{298} = 13.142x10^{-3}T + 90.180x10^{-6}T^{2} - 0.098x10^{2}T^{-1} - 11.902$

Reaction equations (kcal/mol):

298.15-550 K: $ΔHr° = -549.002 - 61.165x10^{-3}T + 84.852x10^{-6}T^{2} - 157.850T^{-1}$
$ΔGr° = -549.002 + 61.165x10^{-3}TlnT - 84.852x10^{-6}T^{2} - 78.925T^{-1} - 20.012x10^{-3}T$

Source: Data from DeKock (112) who estimated all above 298 K.

$Cu_2Se(c)$
Dicopper Selenide
[Reaction: $2Cu(c) + 0.5Se_2(g) = Cu_2Se(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	19.460	31.000	31.000	0	-32.250	-28.091	20.591
300	19.490	31.120	31.000	.036	-32.245	-28.065	20.445
395.4	21.200	36.720	31.736	1.971	-31.917	-26.785	14.805
395.4	19.950	40.840	31.736	3.599	-30.289	-26.785	14.805
400	19.940	41.090	31.843	3.699	-30.268	-26.744	14.612
500	19.890	45.530	34.148	5.691	-30.003	-25.894	11.318
600	19.840	49.160	36.363	7.678	-29.774	-25.098	9.142
700	19.790	52.210	38.410	9.660	-29.575	-24.330	7.596
800	19.740	54.850	40.305	11.636	-29.405	-23.592	6.445
900	19.690	57.170	42.050	13.608	-29.261	-22.873	5.554
1000	19.640	59.250	43.675	15.575	-29.146	-22.178	4.847

Phase change: 395.4 K, α - β transition point of Cu_2Se; ΔH° = 1.628 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-395.4 K: $Cp° = 14.115 + 17.760\times10^{-3}T$
$H°-H°_{298} = 14.115\times10^{-3}T + 8.880\times10^{-6}T^2 - 4.998$
395.4-1.000 K: $Cp° = 20.588 - 0.974\times10^{-3}T - 0.395\times10^5T^{-2}$
$H°-H°_{298} = 20.588\times10^{-3}T - 0.487\times10^{-6}T^2 + 0.395\times10^2T^{-1} - 4.565$

Reaction equations (kcal/mol):

298.15-395.4 K: $\Delta Hr° = -32.302 - 1.857\times10^{-3}T + 7.419\times10^{-6}T^2 - 15.950T^{-1}$
$\Delta Gr° = -32.302 + 1.857\times10^{-3}T\ln T - 7.419\times10^{-6}T^2 - 7.975T^{-1} + 5.845\times10^{-3}T$
395.4-1000 K: $\Delta Hr° = -31.869 + 4.616\times10^{-3}T - 1.948\times10^{-6}T^2 + 23.550T^{-1}$
$\Delta Gr° = -31.869 - 4.616\times10^{-3}T\ln T + 1.948\times10^{-6}T^2 + 11.775T^{-1} + 39.628\times10^{-3}T$

Source: Data from Mills (332).

$CuTe(c)$
Copper Telluride
[Reaction: $Cu(c) + 0.5Te_2(g) = CuTe(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	13.012	20.500	20.500	0	-24.765	-19.291	14.141
300	13.028	20.581	20.501	.024	-24.760	-19.258	14.029
350	13.444	22.625	20.659	.688	-24.610	-18.351	11.459
400	13.882	24.448	21.021	1.371	-24.447	-17.468	9.544
450	14.336	26.110	21.497	2.076	-24.269	-16.608	8.066
500	14.897	27.644	22.036	2.804	-24.074	-15.767	6.892
550	15.844	29.099	22.612	3.568	-23.848	-14.944	5.938
600	17.796	30.555	23.212	4.406	-23.554	-14.147	5.153

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 4.542 + 19.426\times10^{-3}T + 2.380\times10^{5}T^{-2}$

$H°-H°_{298} = 4.542\times10^{-3}T + 9.713\times10^{-6}T^2 - 2.380\times10^{2}T^{-1} - 1.419$

Reaction equations (kcal/mol):

298.15-600 K: $\Delta Hr° = -23.201 - 5.078\times10^{-3}T + 8.606\times10^{-6}T^2 - 243.100T^{-1}$

$\Delta Gr° = -23.201 + 5.078\times10^{-3}T\ln T - 8.606\times10^{-6}T^2 - 121.550T^{-1} - 11.883\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Abbasov (3). Other data from Mills (334).

$Cu_2Te(c)$
Dicopper Telluride
[Reaction: $2Cu(c) + 0.5Te_2(g) = Cu_2Te(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	18.554	28.800	28.800	0	-28.265	-22.903	16.788
300	18.584	28.915	28.802	.034	-28.261	-22.871	16.661
400	20.215	34.484	29.549	1.974	-27.949	-21.117	11.538
440	20.868	36.441	30.087	2.796	-27.790	-20.441	10.153
440	23.064	36.714	30.087	2.916	-27.670	-20.441	10.153
500	23.064	39.661	31.063	4.299	-27.296	-19.482	8.515
526	23.064	40.832	31.516	4.900	-27.135	-19.079	7.927
526	25.552	41.060	31.516	5.020	-27.015	-19.079	7.927
600	31.013	44.625	32.912	7.028	-26.275	-18.005	6.558
600	31.190	45.422	32.912	7.506	-25.797	-18.005	6.558
625	31.190	46.695	33.439	8.285	-25.451	-17.688	6.185
625	24.498	47.690	33.439	8.907	-24.829	-17.688	6.185
700	24.140	50.445	35.115	10.731	-24.315	-16.861	5.264
750	23.901	52.100	36.192	11.932	-23.997	-16.340	4.761
750	22.706	52.739	36.192	12.410	-23.519	-16.340	4.761
800	22.706	54.204	37.273	13.545	-23.276	-15.870	4.335

Phase changes:
440 K, I - II transition point of Cu_2Te; ΔH° = 0.120 kcal/mol.
526 K, II - III transition point of Cu_2Te; ΔH° = 0.120 kcal/mol.
600 K, III - IV transition point of Cu_2Te; ΔH° = 0.478 kcal/mol.
625 K, IV - V transition point of Cu_2Te; ΔH° = 0.622 kcal/mol.
750 K, V - VI transition point of Cu_2Te; ΔH° = 0.478 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-440 K: $Cp° = 13.358 + 16.954\times10^{-3}T + 0.126\times10^{5}T^{-2}$
$H°- H°_{298} = 13.358\times10^{-3}T + 8.477\times10^{-6}T^{2} - 0.126\times10^{2}T^{-1} - 4.694$
440-526 K: $Cp° = 23.064$
$H°- H°_{298} = 23.064\times10^{-3}T - 7.232$
526-600 K: $Cp° = -13.400 + 72.000\times10^{-3}T$
$H°- H°_{298} = -13.400\times10^{-3}T + 36.000\times10^{-6}T^{2} + 2.108$
600-625 K: $Cp° = 31.175$
$H°- H°_{298} = 31.175\times10^{-3}T - 11.199$
625-750 K: $Cp° = 27.777 - 5.066\times10^{-3}T - 0.438\times10^{5}T^{-2}$
$H°- H°_{298} = 27.777\times10^{-3}T - 2.533\times10^{-6}T^{2} + 0.438\times10^{2}T^{-1} - 7.534$
750-800 K: $Cp° = 22.707$
$H°- H°_{298} = 22.707\times10^{-3}T - 4.620$

Reaction equations (kcal/mol):

298.15-440 K: $\Delta Hr° = -28.341 - 1.582\times10^{-3}T + 6.561\times10^{-6}T^{2} - 10.700T^{-1}$
$\Delta Gr° = -28.341 + 1.582\times10^{-3}T\ln T - 6.561\times10^{-6}T^{2} - 5.350T^{-1} + 11.243\times10^{-3}T$
440-526 K: $\Delta Hr° = -30.879 + 8.124\times10^{-3}T - 1.916\times10^{-6}T^{2} + 1.900T^{-1}$
$\Delta Gr° = -30.879 - 8.124\times10^{-3}T\ln T + 1.916\times10^{-6}T^{2} + 0.950T^{-1} + 72.327\times10^{-3}T$
526-600 K: $\Delta Hr° = -21.539 - 28.340\times10^{-3}T + 34.083\times10^{-6}T^{2} + 1.900T^{-1}$
$\Delta Gr° = -21.539 + 28.340\times10^{-3}T\ln T - 34.083\times10^{-6}T^{2} + 0.950T^{-1} - 154.951\times10^{-3}T$
600-625 K: $\Delta Hr° = -34.846 + 16.235\times10^{-3}T - 1.916\times10^{-6}T^{2} + 1.900T^{-1}$
$\Delta Gr° = -34.846 - 16.235\times10^{-3}T\ln T + 1.916\times10^{-6}T^{2} + 0.950T^{-1} + 130.770\times10^{-3}T$
625-750 K: $\Delta Hr° = -31.181 + 12.838\times10^{-3}T - 4.450\times10^{-6}T^{2} + 45.700T^{-1}$
$\Delta Gr° = -31.181 - 12.838\times10^{-3}T\ln T + 4.450\times10^{-6}T^{2} + 22.850T^{-1} + 101.391\times10^{-3}T$
750-800 K: $\Delta Hr° = -28.267 + 7.768\times10^{-3}T - 1.916\times10^{-6}T^{2} + 1.900T^{-1}$
$\Delta Gr° = -28.267 - 7.768\times10^{-3}T\ln T + 1.916\times10^{-6}T^{2} + 0.950T^{-1} + 65.881\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Abbasov (3). Other data from Mills (334).

DyO(g)
Dysprosium Monoxide (ideal gas)
[Formation: Dy(c,l) + 0.5O_2(g) = DyO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	7.590	61.505	61.505	0	-18.000	-23.695	17.369
300	7.590	61.552	61.505	.014	-18.004	-23.731	17.288
400	7.930	63.782	61.807	.790	-18.255	-25.602	13.988
500	8.200	65.583	62.387	1.598	-18.485	-27.411	11.981
600	8.390	67.097	63.050	2.428	-18.708	-29.177	10.627
700	8.520	68.400	63.723	3.274	-18.934	-30.898	9.647
800	8.610	69.544	64.382	4.130	-19.176	-32.595	8.904
900	8.670	70.561	65.012	4.994	-19.437	-34.252	8.317
1000	8.720	71.477	65.613	5.864	-19.724	-35.886	7.843
1100	8.750	72.310	66.185	6.738	-20.048	-37.488	7.448
1200	8.780	73.073	66.728	7.614	-20.423	-39.057	7.113
1300	8.800	73.777	67.243	8.494	-20.857	-40.591	6.824
1400	8.820	74.430	67.734	9.375	-21.359	-42.097	6.572
1500	8.840	75.039	68.200	10.258	-21.937	-43.555	6.346
1600	8.850	75.610	68.646	11.143	-22.597	-44.982	6.144
1657	8.856	75.920	68.891	11.647	-23.013	-45.757	6.035
1657	8.856	75.920	68.891	11.647	-24.008	-45.757	6.035
1682	8.858	76.053	68.996	11.869	-24.064	-46.087	5.988
1682	8.858	76.053	68.996	11.869	-26.707	-46.087	5.988
1700	8.860	76.147	69.072	12.028	-26.841	-46.306	5.953
1800	8.870	76.653	69.479	12.914	-27.592	-47.414	5.757
1900	8.880	77.133	69.869	13.802	-28.344	-48.504	5.579
2000	8.880	77.589	70.244	14.690	-29.099	-49.550	5.415

Phase changes: 1657 K, α - β transition point of Dy; ΔH° = 0.995 kcal/mol.
1682 K, melting point of Dy; ΔH° = 2.643 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.454 + 0.282\times10^{-3}T - 0.843\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 8.454\times10^{-3}T + 0.141\times10^{-6}T^2 + 0.843\times10^{2}T^{-1} - 2.816$

Formation equations (kcal/mol):

298.15-1657 K: $\Delta Hf^\circ = -18.969 + 1.349\times10^{-3}T - 2.335\times10^{-6}T^2 + 230.900T^{-1}$
$\Delta Gf^\circ = -18.969 - 1.349\times10^{-3}T\ln T + 2.335\times10^{-6}T^2 + 115.450T^{-1} - 10.161\times10^{-3}T$
1657-1682 K: $\Delta Hf^\circ = -20.652 - 1.861\times10^{-3}T - 0.110\times10^{-6}T^2 + 61.700T^{-1}$
$\Delta Gf^\circ = -20.652 + 1.861\times10^{-3}T\ln T + 0.110\times10^{-6}T^2 + 30.850T^{-1} - 29.223\times10^{-3}T$
1682-2000 K: $\Delta Hf^\circ = -14.498 - 7.091\times10^{-3}T - 0.110\times10^{-6}T^2 + 61.700T^{-1}$
$\Delta Gf^\circ = -14.498 + 7.091\times10^{-3}T\ln T + 0.110\times10^{-6}T^2 + 30.850T^{-1} - 71.729\times10^{-3}T$

Source: Data from Pedley (396).

ErN(c)
Erbium Nitride
[Formation: $Er(c,l) + 0.5N_2(g) = ErN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.700	18.500	18.500	0	-85.500	-78.978	57.892
300	11.710	18.570	18.503	.020	-85.499	-78.939	57.506
400	11.840	21.960	18.960	1.200	-85.343	-76.771	41.945
500	11.980	24.620	19.840	2.390	-85.188	-74.651	32.630
600	12.110	26.810	20.827	3.590	-85.036	-72.561	26.430
700	12.240	28.690	21.819	4.810	-84.883	-70.489	22.007
800	12.380	30.330	22.780	6.040	-84.743	-68.448	18.699
900	12.520	31.800	23.700	7.290	-84.608	-66.414	16.127
1000	12.650	33.120	24.570	8.550	-84.492	-64.388	14.072
1100	12.780	34.330	25.403	9.820	-84.395	-62.385	12.395
1200	12.920	35.450	26.200	11.100	-84.319	-60.394	10.999
1300	13.060	36.490	26.952	12.400	-84.257	-58.396	9.817
1400	13.190	37.460	27.667	13.710	-84.221	-56.408	8.806
1500	13.320	38.380	28.353	15.040	-84.201	-54.438	7.931
1600	13.460	39.240	29.003	16.380	-84.213	-52.433	7.162
1700	13.600	40.060	29.631	17.730	-84.255	-50.446	6.485
1795	13.723	40.802	30.199	19.031	-84.317	-48.550	5.911
1795	13.723	40.802	30.199	19.031	-89.074	-48.550	5.911
1800	13.730	40.840	30.229	19.100	-89.073	-48.447	5.882
1900	13.860	41.590	30.811	20.480	-89.046	-46.200	5.314
2000	14.000	42.300	31.365	21.870	-89.009	-43.928	4.800

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1795 K, melting point of Er; ΔH° = 4.757 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.300 + 1.350\times10^{-3}T$

$H°-H°_{298} = 11.300\times10^{-3}T + 0.675\times10^{-6}T^2 - 3.429$

Formation equations (kcal/mol):

298.15-1795 K: $\Delta Hf° = -86.461 + 2.761\times10^{-3}T - 0.879\times10^{-6}T^2 + 64.250T^{-1}$

$\Delta Gf° = -86.461 - 2.761\times10^{-3}T\ln T + 0.879\times10^{-6}T^2 + 32.125T^{-1} + 40.208\times10^{-3}T$

1795-2000 K: $\Delta Hf° = -88.115 - 1.209\times10^{-3}T + 0.381\times10^{-6}T^2 + 3.950T^{-1}$

$\Delta Gf° = -88.115 + 1.209\times10^{-3}T\ln T - 0.381\times10^{-6}T^2 + 1.975T^{-1} + 13.652\times10^{-3}T$

Source: Data from Brown (59, 60) who estimated all except enthalpy of formation at 298 K.

ErO(g)
Erbium Monoxide (ideal gas)
[Formation: Er(c,l) + 0.5O_2(g) = ErO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	$C_p°$	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.570	60.913	60.913	0	-10.000	-15.641	11.465
300	7.570	60.960	60.913	.014	-10.005	-15.676	11.420
400	7.930	63.188	61.215	.789	-10.261	-17.526	9.575
500	8.200	64.988	61.794	1.597	-10.501	-19.315	8.442
600	8.390	66.501	62.456	2.427	-10.741	-21.056	7.670
700	8.510	67.804	63.130	3.272	-10.989	-22.753	7.104
800	8.600	68.947	63.787	4.128	-11.250	-24.423	6.672
900	8.670	69.965	64.418	4.992	-11.529	-26.050	6.326
1000	8.720	70.880	65.018	5.862	-11.828	-27.643	6.041
1100	8.750	71.713	65.590	6.735	-12.154	-29.212	5.804
1200	8.780	72.476	66.133	7.612	-12.505	-30.747	5.600
1300	8.800	73.180	66.648	8.491	-12.885	-32.247	5.421
1400	8.820	73.833	67.138	9.373	-13.299	-33.721	5.264
1500	8.840	74.442	67.605	10.256	-13.748	-35.176	5.125
1600	8.850	75.013	68.050	11.140	-14.235	-36.577	4.996
1700	8.860	75.550	68.476	12.026	-14.761	-37.954	4.879
1795	8.870	76.031	68.863	12.868	-15.302	-39.234	4.777
1795	8.870	76.031	68.863	12.868	-20.059	-39.234	4.777
1800	8.870	76.056	68.883	12.912	-20.083	-39.298	4.771
1900	8.870	76.536	69.273	13.799	-20.569	-40.355	4.642
2000	8.880	76.991	69.647	14.687	-21.056	-41.371	4.521

Phase change: 1795 K, melting point of Er; ΔH° = 4.757 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p° = 8.421 + 0.312\times10^{-3}T - 0.839\times10^{5}T^{-2}$
$H°-H°_{298} = 8.421\times10^{-3}T + 0.156\times10^{-6}T^{2} + 0.839\times10^{2}T^{-1} - 2.806$

Formation equations (kcal/mol):

298.15-1795 K: $\Delta Hf° = -10.146 - 0.474\times10^{-3}T - 1.355\times10^{-6}T^{2} + 121.600T^{-1}$
$\Delta Gf° = -10.146 + 0.474\times10^{-3}T\ln T + 1.355\times10^{-6}T^{2} + 60.800T^{-1} - 22.219\times10^{-3}T$
1795-2000 K: $\Delta Hf° = -11.800 - 4.444\times10^{-3}T - 0.095\times10^{-6}T^{2} + 61.300T^{-1}$
$\Delta Gf° = -11.800 + 4.444\times10^{-3}T\ln T + 0.095\times10^{-6}T^{2} + 30.650T^{-1} - 48.775\times10^{-3}T$

Source: Data from Pedley (396).

$Er_6WO_{12}(c)$
Hexaerbium Tungstate
[Formation: $6Er(c) + W(c) + 6O_2(g) = Er_6WO_{12}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	102.500	125.100	125.100	0	-1618.000	-1534.020	1124.453
300	102.600	125.730	125.100	.190	-1617.971	-1533.496	1117.137
400	107.770	156.000	129.200	10.720	-1616.348	-1505.564	822.591
500	111.830	180.500	137.080	21.710	-1614.448	-1478.090	646.064
600	115.450	201.210	146.093	33.070	-1612.388	-1451.023	528.528
700	118.860	219.260	155.274	44.790	-1610.186	-1424.269	444.671
800	122.170	235.350	164.300	56.840	-1607.864	-1397.920	381.889
900	125.410	249.930	173.019	69.220	-1605.425	-1371.799	333.114
930	126.380	254.060	175.566	73.000	-1604.668	-1364.023	320.541
930	90.670	258.040	175.566	76.700	-1600.968	-1364.023	320.541
1000	95.740	264.800	181.580	83.220	-1601.568	-1346.148	294.197
1100	103.000	274.260	189.569	93.160	-1601.989	-1320.576	262.371
1200	110.250	283.540	197.023	103.820	-1601.903	-1295.005	235.850
1300	117.510	292.650	204.027	115.210	-1601.310	-1269.410	213.404
1400	124.760	301.620	210.670	127.330	-1600.237	-1243.898	194.179
1500	132.020	310.480	217.033	140.170	-1598.679	-1218.582	177.545

*Heat capacity at 298 K estimated.

Phase change: 930 K, α - β transition point of Er_6WO_{12}; ΔH° = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-930 K: $Cp° = 98.003 + 31.038x10^{-3}T - 4.238x10^{5}T^{-2}$

$H°- H°_{298} = 98.003x10^{-3}T + 15.519x10^{-6}T^{2} + 4.238x10^{2}T^{-1} - 32.021$

930-1500 K: $Cp° = 23.192 + 72.552x10^{-3}T$

$H°- H°_{298} = 23.192x10^{-3}T + 36.276x10^{-6}T^{2} + 23.756$

Formation equations (kcal/mol):

298.15-930 K: $ΔHf° = -1625.168 + 17.128x10^{-3}T + 4.576x10^{-6}T^{2} + 493.400T^{-1}$

$ΔGf° = -1625.168 - 17.128x10^{-3}T\ln T - 4.576x10^{-6}T^{2} + 246.700T^{-1} + 401.890x10^{-3}T$

930-1500 K: $ΔHf° = -1569.391 - 57.683x10^{-3}T + 25.333x10^{-6}T^{2} + 69.600T^{-1}$

$ΔGf° = -1569.391 + 57.683x10^{-3}T\ln T - 25.333x10^{-6}T^{2} + 34.800T^{-1} - 149.883x10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Levitskii (303). High-temperature data based on Nadiradze (344). Heat capacity at 298 K estimated.

$EuFeO_3(c)$
Europium Ferrite
[Formation: $Eu(c) + Fe(c) + 1.5O_2(g) = EuFeO_3(c)$

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	26.790	25.300	25.300	0	-303.060	-281.197	206.121
300	26.800	25.470	25.303	.050	-303.053	-281.062	204.751
400	27.750	33.280	26.355	2.770	-302.689	-273.781	149.585
500	29.330	39.640	28.400	5.620	-302.297	-266.601	116.530
600	31.150	45.140	30.723	8.650	-301.845	-259.490	94.518
700	33.080	50.090	33.147	11.860	-301.335	-252.473	78.825
800	35.070	54.640	35.565	15.260	-300.766	-245.543	67.078
900	37.100	58.880	37.913	18.870	-300.156	-238.667	57.956
1000	39.160	62.900	40.210	22.690	-299.588	-231.864	50.673

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 17.840 + 21.080\times10^{-3}T + 2.370\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.840\times10^{-3}T + 10.540\times10^{-6}T^{2} - 2.370\times10^{2}T^{-1} - 5.461$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf^\circ = -304.086 + 2.920\times10^{-3}T + 1.434\times10^{-6}T^{2} + 8.300T^{-1}$
$\Delta Gf^\circ = -304.086 - 2.920\times10^{-3}T\ln T - 1.434\times10^{-6}T^{2} + 4.150T^{-1} + 93.787\times10^{-3}T$

Source: Data from Kaul (237).

EuO(g)
Europium Monoxide (ideal gas)
[Formation: $Eu(c,l,g) + 0.5O_2(g) = EuO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.570	61.592	61.592	0	-14.000	-19.513	14.303
300	7.570	61.639	61.592	.014	-14.005	-19.547	14.239
400	7.940	63.869	61.894	.790	-14.248	-21.354	11.667
500	8.210	65.672	62.474	1.599	-14.485	-23.102	10.098
600	8.400	67.187	63.137	2.430	-14.740	-24.801	9.034
700	8.520	68.492	63.812	3.276	-15.021	-26.456	8.260
800	8.610	69.635	64.469	4.133	-15.333	-28.069	7.668
900	8.670	70.653	65.101	4.997	-15.692	-29.639	7.197
1000	8.720	71.570	65.703	5.867	-16.111	-31.167	6.811
1090	8.756	72.322	66.218	6.653	-16.551	-32.503	6.517
1090	8.756	72.322	66.218	6.653	-18.753	-32.503	6.517
1100	8.760	72.402	66.274	6.741	-18.799	-32.629	6.483
1200	8.780	73.165	66.817	7.618	-19.257	-33.865	6.168
1300	8.810	73.869	67.333	8.497	-19.717	-35.064	5.895
1400	8.820	74.523	67.824	9.379	-20.178	-36.228	5.655
1500	8.840	75.132	68.291	10.262	-20.641	-37.357	5.443
1600	8.850	75.703	68.737	11.146	-21.106	-38.457	5.253
1700	8.860	76.240	69.162	12.032	-21.572	-39.527	5.082
1800	8.870	76.747	69.570	12.919	-22.040	-40.573	4.926
1800	8.870	76.747	69.570	12.919	-56.625	-40.573	4.926
1900	8.880	77.226	69.960	13.806	-56.688	-39.674	4.564
2000	8.880	77.682	70.335	14.694	-56.757	-38.778	4.237

Phase changes: 1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.
1800 K, boiling point of Eu; ΔH° = 34.585 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.431 + 0.314\times10^{-3}T - 0.848\times10^{5}T^{-2}$

$H°-H°_{298} = 8.431\times10^{-3}T + 0.157\times10^{-6}T^{2} + 0.848\times10^{2}T^{-1} - 2.812$

Formation equations (kcal/mol):

298.15-1090 K: $\Delta Hf° = -14.436 + 0.520\times10^{-3}T - 2.375\times10^{-6}T^{2} + 146.800T^{-1}$

$\Delta Gf° = -14.436 - 0.520\times10^{-3}T\ln T + 2.375\times10^{-6}T^{2} + 73.400T^{-1} - 15.597\times10^{-3}T$

1090-1800 K: $\Delta Hf° = -14.022 - 4.294\times10^{-3}T - 0.094\times10^{-6}T^{2} + 62.200T^{-1}$

$\Delta Gf° = -14.022 + 4.294\times10^{-3}T\ln T + 0.094\times10^{-6}T^{2} + 31.100T^{-1} - 47.125\times10^{-3}T$

1800-2000 K: $\Delta Hf° = -56.835 + 0.736\times10^{-3}T - 0.350\times10^{-6}T^{2} + 62.200T^{-1}$

$\Delta Gf° = -56.835 - 0.736\times10^{-3}T\ln T + 0.350\times10^{-6}T^{2} + 31.100T^{-1} + 13.904\times10^{-3}T$

Source: Data from Pedley (396).

EuP(c)
Europium Phosphide
[Formation: Eu(c,l,g) + P(c,l,1/4P_4(g)) = EuP(c)]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.640	17.860	17.860	0	-73.200	-70.052	51.348
300*	13.650	17.940	17.873	.020	-73.203	-70.036	51.021
317.3	13.683	18.706	17.898	.256	-73.180	-69.853	48.113
317.3	13.683	18.706	17.898	.256	-73.337	-69.853	48.113
400	13.840	21.900	18.400	1.400	-73.264	-68.948	37.671
500	13.970	25.000	19.420	2.790	-73.183	-67.876	29.668
550	14.020	26.338	19.997	3.488	-73.150	-67.366	26.768
550	14.020	26.338	19.997	3.488	-76.058	-67.366	26.768
600	14.070	27.560	20.577	4.190	-75.947	-66.580	24.251
700	14.160	29.730	21.730	5.600	-75.747	-65.031	20.303
800	14.230	31.630	22.855	7.020	-75.575	-63.516	17.351
900	14.300	33.310	23.921	8.450	-75.443	-62.012	15.058
1000	14.370	34.820	24.940	9.880	-75.374	-60.527	13.228
1090	14.424	36.058	25.805	11.176	-75.365	-59.190	11.868
1090	14.424	36.058	25.805	11.176	-77.567	-59.190	11.868
1100	14.430	36.190	25.899	11.320	-77.563	-59.021	11.726
1200	14.500	37.450	26.808	12.770	-77.513	-57.336	10.442
1300	14.560	38.610	27.672	14.220	-77.464	-55.655	9.356
1400	14.630	39.700	28.500	15.680	-77.406	-53.991	8.428
1500	14.690	40.710	29.277	17.150	-77.339	-52.314	7.622
1600	14.760	41.660	30.023	18.620	-77.272	-50.650	6.918
1700	14.830	42.550	30.726	20.100	-77.196	-48.976	6.296
1800	14.900	43.400	31.406	21.590	-77.110	-47.318	5.745
1800	14.900	43.400	31.406	21.590	-111.695	-47.318	5.745
1900	14.970	44.210	32.063	23.080	-111.202	-43.760	5.033
2000	15.050	44.980	32.690	24.580	-110.702	-40.224	4.395

*Data above 298 K estimated.

Phase changes:
317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to P_4(g); ΔH° = 2.908 kcal/mol of P.
1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.
1800 K, boiling point of Eu; ΔH° = 34.585 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2200 K:
$Cp^\circ = 13.747 + 0.646\times10^{-3}T - 0.266\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 13.747\times10^{-3}T + 0.323\times10^{-6}T^2 + 0.266\times10^{2}T^{-1} - 4.217$

Formation equations (kcal/mol):

298.15-317.3 K:
$\Delta Hf^\circ = -74.801 + 5.652\times10^{-3}T - 5.142\times10^{-6}T^2 + 111.200T^{-1}$
$\Delta Gf^\circ = -74.801 - 5.652\times10^{-3}T\ln T + 5.142\times10^{-6}T^2 + 55.600T^{-1} + 45.974\times10^{-3}T$

317.3-550 K:
$\Delta Hf^\circ = -74.488 + 3.159\times10^{-3}T - 1.957\times10^{-6}T^2 + 111.200T^{-1}$
$\Delta Gf^\circ = -74.488 - 3.159\times10^{-3}T\ln T + 1.957\times10^{-6}T^2 + 55.600T^{-1} + 31.638\times10^{-3}T$

550-1090 K:
$\Delta Hf^\circ = -77.948 + 4.497\times10^{-3}T - 1.961\times10^{-6}T^2 + 10.900T^{-1}$
$\Delta Gf^\circ = -77.948 - 4.497\times10^{-3}T\ln T + 1.961\times10^{-6}T^2 + 5.450T^{-1} + 46.536\times10^{-3}T$

1090-1800 K:
$\Delta Hf^\circ = -77.534 - 0.317\times10^{-3}T + 0.319\times10^{-6}T^2 - 73.700T^{-1}$
$\Delta Gf^\circ = -77.534 + 0.317\times10^{-3}T\ln T - 0.319\times10^{-6}T^2 - 36.850T^{-1} + 15.008\times10^{-3}T$

1800-2000 K:
$\Delta Hf^\circ = -120.347 + 4.713\times10^{-3}T + 0.064\times10^{-6}T^2 - 73.700T^{-1}$
$\Delta Gf^\circ = -120.347 - 4.713\times10^{-3}T\ln T - 0.064\times10^{-6}T^2 - 36.850T^{-1} + 76.036\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Gordienko (180). Low-temperature heat capacities and entropy at 298 K from Mironov (335). High-temperature data are those estimated by Gordienko (180).

$EuSe(c)$
Europium Selenide
[Reaction: $Eu(c,l) + 0.5Se_2(g) = EuSe(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	11.680	25.430	25.430	0	-110.450	-103.810	76.094
300	11.690	25.500	25.433	.020	-110.451	-103.770	75.595
400	11.980	28.910	25.910	1.200	-110.434	-101.550	55.484
500	12.230	31.610	26.770	2.420	-110.398	-99.321	43.413
600	12.470	33.860	27.777	3.650	-110.381	-97.113	35.373
700	12.700	35.800	28.786	4.910	-110.364	-94.900	29.629
800	12.930	37.510	29.772	6.190	-110.358	-92.690	25.321
900	13.150	39.040	30.707	7.500	-110.366	-90.471	21.969
1000	13.370	40.440	31.620	8.820	-110.422	-88.267	19.291
1090	13.568	41.606	32.400	10.034	-110.504	-86.273	17.298
1090	13.568	41.606	32.400	10.034	-112.706	-86.273	17.298
1100	13.590	41.730	32.485	10.170	-112.711	-86.031	17.093
1200	13.820	42.920	33.303	11.540	-112.746	-83.601	15.226
1300	14.040	44.030	34.084	12.930	-112.758	-81.165	13.645
1400	14.260	45.080	34.830	14.350	-112.738	-78.736	12.291
1500	14.480	46.070	35.550	15.780	-112.704	-76.313	11.119
1600	14.700	47.010	36.235	17.240	-112.638	-73.887	10.092
1700	14.920	47.910	36.898	18.720	-112.548	-71.466	9.187

*Entropy at 298 K estimated.

Phase change: 1090 K, melting point of Eu; $\Delta H^\circ = 2.202$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1700 K: $Cp^\circ = 11.195 + 2.192\times10^{-3}T - 0.150\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 11.195\times10^{-3}T + 1.096\times10^{-6}T^{2} + 0.150\times10^{2}T^{-1} - 3.486$

Reaction equations (kcal/mol):

298.15-1090 K: $\Delta Hr^\circ = -111.060 + 1.567\times10^{-3}T - 1.025\times10^{-6}T^{2} + 69.650T^{-1}$
$\Delta Gr^\circ = -111.060 - 1.567\times10^{-3}T\ln T + 1.025\times10^{-6}T^{2} + 34.825T^{-1} + 32.546\times10^{-3}T$
1090-1700 K: $\Delta Hr^\circ = -110.646 - 3.247\times10^{-3}T + 1.256\times10^{-6}T^{2} - 14.950T^{-1}$
$\Delta Gr^\circ = -110.646 + 3.247\times10^{-3}T\ln T - 1.256\times10^{-6}T^{2} - 7.475T^{-1} + 1.018\times10^{-3}T$

Source: Data based on McMasters (327) who estimated entropy at 298 K.

EuTe(c)
Europium Telluride
[Reaction: Eu(c,l) + 0.5Te_2(g) = EuTe(c)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	11.780	27.170	27.170	0	-112.365	-105.697	77.477
300	11.790	27.240	27.173	.020	-112.365	-105.657	76.970
400	12.150	30.690	27.640	1.220	-112.270	-103.432	56.512
500	12.430	33.430	28.530	2.450	-112.168	-101.231	44.247
600	12.670	35.720	29.537	3.710	-112.072	-99.047	36.077
700	12.900	37.690	30.576	4.980	-112.004	-96.890	30.250
800	13.120	39.430	31.580	6.280	-111.948	-94.740	25.881
900	13.330	40.980	32.524	7.610	-111.914	-92.577	22.480
1000	13.540	42.400	33.450	8.950	-111.939	-90.435	19.764
1090	13.729	43.575	34.233	10.183	-112.002	-88.490	17.742
1090	13.729	43.575	34.233	10.183	-114.204	-88.490	17.742
1100	13.750	43.700	34.318	10.320	-114.207	-88.254	17.534
1200	13.950	44.900	35.150	11.700	-114.243	-85.891	15.643
1300	14.160	46.030	35.945	13.110	-114.257	-83.529	14.042
1400	14.370	47.090	36.711	14.530	-114.269	-81.177	12.672
1500	14.570	48.080	37.427	15.980	-114.252	-78.798	11.481
1600	14.770	49.030	38.124	17.450	-114.215	-76.441	10.441
1700	14.980	49.930	38.795	18.930	-114.167	-74.079	9.523

*Entropy at 298 K estimated.

Phase change: 1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1700 K: $Cp° = 11.548 + 2.024 \times 10^{-3}T - 0.326 \times 10^{5}T^{-2}$
$H° - H°_{298} = 11.548 \times 10^{-3}T + 1.012 \times 10^{-6}T^{2} + 0.326 \times 10^{2}T^{-1} - 3.642$

Reaction equations (kcal/mol):

298.15-1090 K: $\Delta Hr° = -113.459 + 2.953 \times 10^{-3}T - 1.565 \times 10^{-6}T^{2} + 105.100T^{-1}$
$\Delta Gr° = -113.459 - 2.953 \times 10^{-3}T\ln T + 1.565 \times 10^{-6}T^{2} + 52.550T^{-1} + 41.798 \times 10^{-3}T$
1090-1700 K: $\Delta Hr° = -113.045 - 1.861 \times 10^{-3}T + 0.715 \times 10^{-6}T^{2} + 20.500T^{-1}$
$\Delta Gr° = -113.045 + 1.861 \times 10^{-3}T\ln T - 0.715 \times 10^{-6}T^{2} + 10.250T^{-1} + 10.270 \times 10^{-3}T$

Source: Data based on McMasters (327) who estimated entropy at 298 K.

$Eu_6WO_{12}(c)$
Hexaeuropium Tungstate
[Formation: $6Eu(c,l) + W(c) + 6O_2(g) = Eu_6WO_{12}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	102.700	115.000	115.000	0	-1440.000	-1351.023	990.314
300	103.060	115.640	115.007	.190	-1439.971	-1350.469	983.803
400	116.690	147.400	119.250	11.260	-1437.742	-1320.928	721.712
500	123.870	174.280	127.640	23.320	-1434.754	-1292.052	564.748
600	128.510	197.300	137.367	35.960	-1431.510	-1263.806	460.335
700	131.960	217.380	147.394	48.990	-1428.202	-1236.109	385.926
800	134.760	235.190	157.278	62.330	-1424.902	-1208.902	330.252
900	137.190	251.200	166.833	75.930	-1421.723	-1182.080	287.045
1000	139.400	265.770	176.010	89.760	-1418.756	-1155.612	252.556
1090	141.245	277.869	183.937	102.387	-1416.339	-1132.040	226.976
1090	141.245	277.869	183.937	102.387	-1429.551	-1132.040	226.976
1100	141.450	279.160	184.796	103.800	-1429.255	-1129.314	224.371
1200	143.400	291.550	193.183	118.040	-1426.231	-1102.183	200.732
1300	145.270	303.100	201.192	132.480	-1423.062	-1075.286	180.770
1400	147.100	313.930	208.859	147.100	-1419.771	-1048.645	163.699
1500	148.880	324.140	216.207	161.900	-1416.343	-1022.257	148.941

*Heat capacity at 298 K estimated.

Phase change: 1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 125.633 + 16.234\times10^{-3}T - 24.694\times10^{5}T^{-2}$

$H° - H°_{298} = 125.633\times10^{-3}T + 8.117\times10^{-6}T^{2} + 24.694\times10^{2}T^{-1} - 46.461$

Formation equations (kcal/mol):

298.15-1090 K: $\Delta Hf° = -1463.314 + 50.662\times10^{-3}T - 8.952\times10^{-6}T^{2} + 2684.800T^{-1}$

$\Delta Gf° = -1463.314 - 50.662\times10^{-3}T\ln T + 8.952\times10^{-6}T^{2} + 1342.400T^{-1} + 647.507\times10^{-3}T$

1090-1500 K: $\Delta Hf° = -1460.830 + 21.778\times10^{-3}T + 4.728\times10^{-6}T^{2} + 2177.200T^{-1}$

$\Delta Gf° = -1460.830 - 21.778\times10^{-3}T\ln T - 4.728\times10^{-6}T^{2} + 1088.600T^{-1} + 458.340\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Levitskii (303). High-temperature data based on Nadiradze (343). Heat capacity at 298 K estimated.

$FeAl_2O_4(c)$
Iron Aluminate
[Formation: $Fe(c) + 2Al(c,l) + 2O_2(g) = FeAl_2O_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	29.530	25.400	25.400	0	-470.000	-442.367	324.259
300*	29.640	25.580	25.413	.050	-470.009	-442.199	322.138
400	34.000	34.770	26.620	3.260	-470.041	-432.911	236.529
500	36.630	42.660	29.060	6.800	-469.893	-423.644	185.172
600	38.400	49.500	31.900	10.560	-469.682	-414.404	150.945
700	39.700	55.520	34.863	14.460	-469.497	-405.212	126.511
800	40.700	60.890	37.778	18.490	-469.366	-396.035	108.190
900	41.530	65.740	40.629	22.600	-469.366	-386.879	93.946
933.61	41.765	67.267	41.561	24.000	-469,410	-383.798	89.843
933.61	41.765	67.267	41.561	24.000	-474.570	-383.798	89.843
1000	42.230	70.150	43.360	26.790	-474.666	-377.338	82.466
1043	42.501	71.934	44.502	28.612	-474.850	-373.150	78.189
1100	42.860	74.200	45.982	31.040	-474.944	-367.587	73.032
1185	43.345	77.414	48.124	34.709	-474.890	-359.293	66.264
1185	43.345	77.414	48.124	34.709	-475.105	-359.293	66.264
1200	43.430	77.960	48.493	35.360	-475.059	-357.829	65.169
1300	43.960	81.460	50.898	39.730	-474.739	-348.076	58.516
1400	44.480	84.730	53.194	44.150	-474.406	-338.337	52.816
1500	44.980	87.820	55.407	48.620	-474.055	-328.642	47.882

*Data above 298 K estimated.

Phase changes: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 36.670 + 6.328\times10^{-3}T - 8.024\times10^{5}T^{-2}$
$H°-H°_{298} = 36.670\times10^{-3}T + 3.164\times10^{-6}T^{2} + 8.024\times10^{2}T^{-1} - 13.906$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -476.566 + 13.247\times10^{-3}T - 7.367\times10^{-6}T^{2} + 975.300T^{-1}$
$\Delta Gf° = -476.566 - 13.247\times10^{-3}T\ln T + 7.367\times10^{-6}T^{2} + 487.650T^{-1} + 182.498\times10^{-3}T$
933.61-1043 K: $\Delta Hf° = -479.101 + 7.251\times10^{-3}T - 3.913\times10^{-6}T^{2} + 940.500T^{-1}$
$\Delta Gf° = -479.101 - 7.251\times10^{-3}T\ln T + 3.913\times10^{-6}T^{2} + 470.250T^{-1} + 147.451\times10^{-3}T$
1043-1185 K: $\Delta Hf° = -455.540 - 36.730\times10^{-3}T + 16.798\times10^{-6}T^{2} + 712.000T^{-1}$
$\Delta Gf° = -455.540 + 36.730\times10^{-3}T\ln T - 16.798\times10^{-6}T^{2} + 356.000T^{-1} - 159.093\times10^{-3}T$
1185-1500 K: $\Delta Hf° = -479.154 + 1.525\times10^{-3}T + 1.107\times10^{-6}T^{2} + 831.000T^{-1}$
$\Delta Gf° = -479.154 - 1.525\times10^{-3}T\ln T - 1.107\times10^{-6}T^{2} + 415.500T^{-1} + 112.948\times10^{-3}T$

Source: Enthalpy of formation at 298 K from Wagman (514). Low-temperature heat capacities and entropy at 298 K from King (262). High-temperature data estimated.

FeB(c,l)
Iron Boride
[Formation: Fe(c,l) + B(β) = FeB(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	9.810	8.600	8.600	0	-14.220	-14.420	10.570
300	9.850	8.660	8.600	.020	-14.216	-14.418	10.503
400	11.320	11.730	9.030	1.080	-14.099	-14.517	7.932
500	12.130	14.350	9.830	2.260	-14.008	-14.627	6.393
600	12.680	16.610	10.777	3.500	-13.980	-14.756	5.375
700	13.110	18.600	11.757	4.790	-14.003	-14.884	4.647
800	13.470	20.370	12.720	6.120	-14.084	-15.001	4.098
900	13.790	21.980	13.669	7.480	-14.255	-15.114	3.670
1000	14.090	23.440	14.560	8.880	-14.579	-15.179	3.317
1043	14.210	24.036	14.938	9.488	-14.862	-15.200	3.185
1100	14.370	24.800	15.436	10.300	-15.095	-15.224	3.025
1185	14.600	25.876	16.146	11.531	-15.274	-15.223	2.808
1185	14.600	25.876	16.146	11.531	-15.489	-15.223	2.808
1200	14.640	26.060	16.268	11.750	-15.485	-15.221	2.772
1300	14.910	27.240	17.063	13.230	-15.459	-15.190	2.554
1400	15.170	28.360	17.839	14.730	-15.448	-15.182	2.370
1500	15.420	29.410	18.570	16.260	-15.442	-15.151	2.207
1600	15.670	30.420	19.283	17.820	-15.441	-15.148	2.069
1667	15.837	31.069	19.745	18.876	-15.449	-15.140	1.985
1667	15.837	31.069	19.745	18.876	-15.649	-15.140	1.985
1700	15.920	31.380	19.968	19.400	-15.680	-15.129	1.945
1800	16.170	32.290	20.623	21.000	-15.786	-15.073	1.830
1811	16.198	32.389	20.694	21.178	-15.801	-15.072	1.819
1811	16.198	32.389	20.694	21.178	-19.101	-15.072	1.819
1900	16.420	33.170	21.259	22.630	-19.270	-14.866	1.710
1931	16.500	33.440	21.457	23.140	-19.327	-14.801	1.675
1931	21.510	41.200	21.459	38.120	-4.347	-14.805	1.676
2000	21.510	41.950	22.150	39.600	-4.134	-15.190	1.660

Phase changes:
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.
1931 K, melting point of FeB; ΔH° = 14.980 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1931 K: $Cp^\circ = 11.950 + 2.388\times10^{-3}T - 2.533\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 11.950\times10^{-3}T + 1.194\times10^{-6}T^{2} + 2.533\times10^{2}T^{-1} - 4.519$
1931-2000 K: $Cp^\circ = 21.510$
$H^\circ - H^\circ_{298} = 21.510\times10^{-3}T - 3.416$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -16.819 + 7.448\times10^{-3}T - 5.569\times10^{-6}T^{2} + 260.300T^{-1}$
$\Delta Gf^\circ = -16.819 - 7.448\times10^{-3}T\ln T + 5.569\times10^{-6}T^{2} + 130.150T^{-1} + 47.357\times10^{-3}T$
1043-1185 K: $\Delta Hf^\circ = 6.742 - 36.533\times10^{-3}T + 15.142\times10^{-6}T^{2} + 31.800T^{-1}$
$\Delta Gf^\circ = 6.742 + 36.533\times10^{-3}T\ln T - 15.142\times10^{-6}T^{2} + 15.900T^{-1} - 259.188\times10^{-3}T$
1185-1667 K: $\Delta Hf^\circ = -16.872 + 1.722\times10^{-3}T - 0.549\times10^{-6}T^{2} + 150.800T^{-1}$
$\Delta Gf^\circ = -16.872 - 1.722\times10^{-3}T\ln T + 0.549\times10^{-6}T^{2} + 75.400T^{-1} + 12.853\times10^{-3}T$
1667-1811 K: $\Delta Hf^\circ = -99.767 + 50.219\times10^{-3}T - 10.180\times10^{-6}T^{2} + 47850\ T^{-1}$
$\Delta Gf^\circ = -99.767 - 50.219\times10^{-3}T\ln T + 10.180\times10^{-6}T^{2} + 23925.000T^{-1} + 397.732\times10^{-3}T$
1811-1931 K: $\Delta Hf^\circ = -13.917 - 3.773\times10^{-3}T + 0.502\times10^{-6}T^{2} + 31.800T^{-1}$
$\Delta Gf^\circ = -13.917 + 3.773\times10^{-3}T\ln T - 0.502\times10^{-6}T^{2} + 15.900T^{-1} - 28.066\times10^{-3}T$
1931-2000 K: $\Delta Hf^\circ = -12.814 + 5.787\times10^{-3}T - 0.692\times10^{-6}T^{2} - 221.500T^{-1}$
$\Delta Gf^\circ = -12.814 - 5.787\times10^{-3}T\ln T + 0.692\times10^{-6}T^{2} - 110.750T^{-1} + 41.420\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Sato (435). Other data from Chart (79).

$Fe_2B(c)$
Diiron Boride
[Formation: $2Fe(c) + B(\beta) = Fe_2B(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.960	16.600	16.600	0	-13.300	-13.941	10.219
300	16.020	16.700	16.600	.030	-13.297	-13.944	10.158
400	18.060	21.620	17.270	1.740	-13.156	-14.189	7.752
500	19.180	25.780	18.560	3.610	-13.057	-14.454	6.318
600	19.950	29.350	20.067	5.570	-13.046	-14.737	5.368
700	20.540	32.470	21.613	7.600	-13.124	-15.006	4.685
800	21.050	35.250	23.150	9.680	-13.320	-15.266	4.170
900	21.500	37.750	24.639	11.800	-13.693	-15.491	3.762
1000	21.920	40.040	26.060	13.980	-14.373	-15.653	3.421
1043	22.092	40.966	26.656	14.926	-14.953	-15.697	3.289
1100	22.320	42.150	27.432	16.190	-15.431	-15.732	3.126
1185	22.651	43.825	28.551	18.100	-15.814	-15.742	2.903
1185	22.651	43.825	28.551	18.100	-16.244	-15.742	2.903
1200	22.710	44.110	28.743	18.440	-16.242	-15.738	2.866
1300	23.080	45.940	29.994	20.730	-16.226	-15.688	2.637
1400	23.450	47.670	31.199	23.060	-16.226	-15.652	2.443
1500	23.810	49.300	32.353	25.420	-16.251	-15.609	2.274
1600	24.160	50.840	33.452	27.820	-16.291	-15.561	2.126

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, $\alpha \rightarrow \gamma$ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp^\circ = 18.893 + 3.380\times10^{-3}T - 3.499\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 18.893\times10^{-3}T + 1.690\times10^{-6}T^{2} + 3.499\times10^{2}T^{-1} - 6.957$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -18.629 + 14.612\times10^{-3}T - 11.144\times10^{-6}T^{2} + 585.400T^{-1}$
$\Delta Gf^\circ = -18.629 - 14.612\times10^{-3}T\ln T + 11.144\times10^{-6}T^{2} + 292.700T^{-1} + 92.363\times10^{-3}T$
1043-1185 K: $\Delta Hf^\circ = 28.492 - 73.350\times10^{-3}T + 30.278\times10^{-6}T^{2} + 128.400T^{-1}$
$\Delta Gf^\circ = 28.492 + 73.350\times10^{-3}T\ln T - 30.278\times10^{-6}T^{2} + 64.200T^{-1} - 520.726\times10^{-3}T$
1185-1600 K: $\Delta Hf^\circ = -18.736 + 3.160\times10^{-3}T - 1.104\times10^{-6}T^{2} + 366.400T^{-1}$
$\Delta Gf^\circ = -18.736 - 3.160\times10^{-3}T\ln T + 1.104\times10^{-6}T^{2} + 183.200T^{-1} + 23.356\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Sato (435). Other data from Chart (79).

$Fe_3C(c)$
Triiron Carbide, Cementite
[Formation: $3Fe(c,l) + C(c) = Fe_3C(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	25.400	25.000	25.000	0	5.985	4.772	-3.498
300	25.440	25.160	25.003	.047	5.995	4.764	-3.470
400	27.930	32.800	26.025	2.710	6.536	4.274	-2.335
478	30.710	38.170	27.601	5.052	7.055	3.772	-1.725
478	26.350	38.170	27.601	5.052	7.055	3.772	-1.725
500	26.500	39.340	28.092	5.624	7.087	3.620	-1.582
600	27.200	44.230	30.382	8.309	7.184	2.919	-1.063
700	27.900	48.480	32.674	11.064	7.130	2.208	-.689
800	28.600	52.250	34.889	13.889	6.901	1.518	-.415
900	29.300	55.660	37.011	16.784	6.423	.869	-.211
1000	30	58.780	39.031	19.749	5.473	.298	-.065
1043*	30.301	60.049	39.872	21.045	4.644	.091	-.019
1100	30.700	61.680	40.967	22.784	3.988	-.134	.027
1185	31.295	63.986	42.535	25.419	3.514	-.443	.082
1185	31.295	63.986	42.535	25.419	2.869	-.443	.082
1200	31.400	64.380	42.806	25.889	2.892	-.488	.089
1300	32.100	66.920	44.563	29.064	3.057	-.773	.130
1400	32.800	69.320	46.242	32.309	3.220	-1.068	.167
1500	33.500	71.610	47.861	35.624	3.384	-1.384	.202

*Data extrapolated above 1000 K.

Phase changes: 478 K, Curie temperature of Fe_3C; ΔH° = 0 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-478 K: $Cp^\circ = -0.592 + 61.700\times10^{-3}T + 6.753\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = -0.592\times10^{-3}T + 30.850\times10^{-6}T^2 - 6.753\times10^{2}T^{-1} - 0.301$
478-1500 K: $Cp^\circ = 22.567 + 7.352\times10^{-3}T + 0.613\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 22.567\times10^{-3}T + 3.676\times10^{-6}T^2 - 0.613\times10^{2}T^{-1} - 6.447$

Formation equations (kcal/mol):

298.15-478 K: $\Delta Hf^\circ = 6.501 - 3.447\times10^{-3}T + 11.871\times10^{-6}T^2 - 162.100T^{-1}$
$\Delta Gf^\circ = 6.501 + 3.447\times10^{-3}T\ln T - 11.871\times10^{-6}T^2 - 81.050T^{-1} - 20.988\times10^{-3}T$
478-1043 K: $\Delta Hf^\circ = 0.355 + 19.712\times10^{-3}T - 15.303\times10^{-6}T^2 + 451.900T^{-1}$
$\Delta Gf^\circ = 0.355 - 19.712\times10^{-3}T\ln T + 15.303\times10^{-6}T^2 + 225.950T^{-1} + 120.419\times10^{-3}T$
1043-1185 K: $\Delta Hf^\circ = 71.038 - 112.231\times10^{-3}T + 46.830\times10^{-6}T^2 - 233.600T^{-1}$
$\Delta Gf^\circ = 71.038 + 112.231\times10^{-3}T\ln T - 46.830\times10^{-6}T^2 - 116.800T^{-1} - 799.215\times10^{-3}T$
1185-1500 K: $\Delta Hf^\circ = 0.196 + 2.534\times10^{-3}T - 0.243\times10^{-6}T^2 + 123.400T^{-1}$
$\Delta Gf^\circ = 0.196 - 2.534\times10^{-3}T\ln T + 0.243\times10^{-6}T^2 + 61.700T^{-1} + 16.907\times10^{-3}T$

Source: Data to 1000 K from Chipman (90). Data above 1000 K extrapolated.

$FeCO_3(c)$
Iron Carbonate
[Formation: $Fe(c) + C(c) + 1.5O_2(g) = FeCO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	20.440	22.970	22.970	0	-177.320	-159.899	117.208
300*	20.490	23.100	22.973	.038	-177.317	-159.792	116.407
400	23.170	29.370	23.818	2.221	-177.069	-153.988	84.134
500	25.850	34.840	25.498	4.671	-176.714	-148.263	64.805
600	28.530	39.800	27.483	7.390	-176.242	-142.620	51.949
700	31.210	44.400	29.576	10.377	-175.641	-137.063	42.792
800	33.890	48.750	31.711	13.631	-174.908	-131.609	35.953

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 12.447 + 26.796\text{x}10^{-3}T + 0.003\text{x}10^{5}T^{-2}$
$H°- H°_{298} = 12.447\text{x}10^{-3}T + 13.398\text{x}10^{-6}T^{2} - 0.003\text{x}10^{2}T^{-1} - 4.901$

Formation equations (kcal/mol):

298.15-800 K: $\Delta Hf° = -177.291 - 1.695\text{x}10^{-3}T + 5.807\text{x}10^{-6}T^{2} - 11.900T^{-1}$
$\Delta Gf° = -177.291 + 1.695\text{x}10^{-3}T\ln T - 5.807\text{x}10^{-6}T^{2} - 5.950T^{-1} + 50.473\text{x}10^{-3}T$

Source: Data from Chang (74) who estimated all above 298 K.

$Fe(CO)_5(g)$
Iron Pentacarbonyl (ideal gas)
[Formation: $Fe(c) + 5C(c) + 2.5O_2(g) = Fe(CO)_5(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	40.790	104.960	104.960	0	-175.200	-165.977	121.663
300	40.900	105.210	104.960	.076	-175.188	-165.919	120.870
400	45.160	117.610	106.620	4.396	-174.488	-162.935	89.022
500	47.950	128.010	109.892	9.059	-173.920	-160.120	69.987
600	50.080	136.950	113.675	13.965	-173.523	-157.396	57.331
700	51.810	144.800	117.569	19.062	-173.286	-154.729	48.308
800	53.230	151.810	121.415	24.316	-173.188	-152.084	41.547
900	54.410	158.150	125.150	29.700	-173.236	-149.450	36.291
1000	55.390	163.940	128.748	35.192	-173.482	-146.802	32.083

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 44.812 + 11.654x10^{-3}T - 6.665x10^{5}T^{-2}$

$H°-H°_{298} = 44.812x10^{-3}T + 5.827x10^{-6}T^{2} + 6.665x10^{2}T^{-1} - 16.114$

Formation equations (kcal/mol):

298.15-1000 K: $ΔHf° = -177.252 + 9.368x10^{-3}T - 5.332x10^{-6}T^{2} - 79.500T^{-1}$

$ΔGf° = -177.252 - 9.368x10^{-3}TlnT + 5.332x10^{-6}T^{2} - 39.750T^{-1} + 90.049x10^{-3}T$

Source: Data from Behrens (26).

$FeCr_2O_4(c)$
Iron Chromate

[Formation: $Fe(c,l) + 2Cr(c) + 2O_2(g) = FeCr_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	31.940	34.900	34.900	0	-345.300	-321.171	235.421
300	32.046	35.098	34.901	.059	-345.298	-321.023	233.862
311.5	32.519	36.312	34.931	.430	-345.292	-320.092	224.575
400	36.155	44.959	36.216	3.497	-345.068	-312.958	170.990
500	38.448	53.292	38.822	7.235	-344.718	-304.967	133.299
600	40.029	60.449	41.844	11.163	-344.353	-297.048	108.198
700	41.245	66.715	44.959	15.229	-344.012	-289.189	90.288
800	42.240	72.289	48.033	19.405	-343.721	-281.381	76.869
900	43.084	77.314	51.012	23.672	-343.504	-273.601	66.439
1000	43.814	81.892	53.874	28.018	-343.452	-265.844	58.099
1043	44.087	83.742	55.068	29.908	-343.581	-262.505	55.004
1100	44.450	86.099	56.615	32.432	-343.620	-258.069	51.273
1185	44.922	89.425	58.851	36.231	-343.540	-251.453	46.375
1185	44.922	89.425	58.851	36.231	-343.755	-251.453	46.375
1200	45.005	89.991	59.237	36.905	-343.712	-250.286	45.583
1300	45.486	93.612	61.743	41.430	-343.461	-242.528	40.772
1400	45.899	96.999	64.142	46.000	-343.278	-234.782	36.651
1500	46.247	100.178	66.439	50.608	-343.163	-227.015	33.076
1600	46.533	103.172	68.643	55.247	-343.143	-219.273	29.951
1667	46.684	105.084	70.069	58.370	-343.179	-214.107	28.070
1667	46.684	105.084	70.069	58.370	-343.379	-214.107	28.070
1700	46.758	106.000	70.758	59.912	-343.437	-211.548	27.196
1800	46.924	108.678	72.791	64.597	-343.676	-203.758	24.739
1811	46.936	108.964	73.010	65.113	-343.711	-202.906	24.486
1811	46.936	108.964	73.010	65.113	-347.011	-202.906	24.486
1900	47.031	111.218	74.747	69.295	-347.390	-195.827	22.525
2000	47.081	113.632	76.632	74.001	-347.874	-187.830	20.525

Phase changes:
311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α − γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ − δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 39.442 + 4.800\times10^{-3}T - 7.860\times10^{5}T^{-2}$
$H°- H°_{298} = 39.442\times10^{-3}T + 2.400\times10^{-6}T^{2} + 7.860\times10^{2}T^{-1} - 14.609$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -354.671 + 30.819\times10^{-3}T - 32.811\times10^{-6}T^{2} + 924.100T^{-1}$
$\Delta Gf° = -354.671 - 30.819\times10^{-3}T\ln T + 32.811\times10^{-6}T^{2} + 462.050T^{-1} + 272.976\times10^{-3}T$
311.5-1043 K: $\Delta Hf° = -352.676 + 16.485\times10^{-3}T - 8.259\times10^{-6}T^{2} + 951.300T^{-1}$
$\Delta Gf° = -352.676 - 16.485\times10^{-3}T\ln T + 8.259\times10^{-6}T^{2} + 475.650T^{-1} + 191.781\times10^{-3}T$
1043-1185 K: $\Delta Hf° = -329.115 - 27.496\times10^{-3}T + 12.452\times10^{-6}T^{2} + 722.800T^{-1}$
$\Delta Gf° = -329.115 + 27.496\times10^{-3}T\ln T - 12.452\times10^{-6}T^{2} + 361.400T^{-1} - 114.764\times10^{-3}T$
1185-1667 K: $\Delta Hf° = -352.729 + 10.759\times10^{-3}T - 3.239\times10^{-6}T^{2} + 841.800T^{-1}$
$\Delta Gf° = -352.729 - 10.759\times10^{-3}T\ln T + 3.239\times10^{-6}T^{2} + 420.900T^{-1} + 157.277\times10^{-3}T$
1667-1811 K: $\Delta Hf° = -435.624 + 59.256\times10^{-3}T - 12.870\times10^{-6}T^{2} + 48541.000T^{-1}$
$\Delta Gf° = -435.624 - 59.256\times10^{-3}T\ln T + 12.870\times10^{-6}T^{2} + 24270.500T^{-1} + 542.155\times10^{-3}T$
1811-2000 K: $\Delta Hf° = -349.774 + 5.264\times10^{-3}T - 2.188\times10^{-6}T^{2} + 722.800T^{-1}$
$\Delta Gf° = -349.774 - 5.264\times10^{-3}T\ln T + 2.188\times10^{-6}T^{2} + 361.400T^{-1} + 116.357\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Low-temperature heat capacities and entropy at 298 K from Shomate (449). High-temperature data based on Naylor (350).

$(Fe^{+2}_{5.2766}Mg_{1.5209}Fe^{+3}_{0.12}Mn_{0.0825})(Si_{7.9163}Al_{0.0837}O_{22.0363})(OH)_{1.9637}(c)$

Amosite

[Formation: $5.3966Fe(c) + 1.5209Mg(c,l) + 0.0825Mn(c) + 7.9163Si(c) + 0.0837Al(c,l) + 12O_2(g) + 0.98185H_2(g) = \text{Amosite}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	162.800	168.800	168.800	0	-2419.200	-2260.052	1656.641
300	163.300	169.800	168.800	.300	-2419.218	-2259.060	1645.703
400	189.800	220.500	175.500	18.000	-2419.143	-2205.643	1205.092
500	209.600	265.100	189.060	38.020	-2417.666	-2152.409	940.805
600	223.500	304.600	205.083	59.710	-2415.357	-2099.562	764.755
700	233.400	339.900	221.929	82.580	-2412.658	-2047.185	639.152
800	241.100	371.600	238.725	106.300	-2409.890	-1995.201	545.056
900	247.300	400.300	254.967	130.800	-2407.232	-1943.380	471.911
922	248.246	406.284	258.506	136.251	-2406.736	-1932.054	457.966
922	248.246	406.284	258.506	136.251	-2409.990	-1932.054	457.966
933.61	248.745	409.393	260.363	139.136	-2409.753	-1926.037	450.862
933.61	248.745	409.393	260.363	139.136	-2409.969	-1926.037	450.862
980	250.740	421.526	267.774	150.677	-2409.101	-1902.029	424.166
980	250.740	421.526	267.774	150.677	-2409.145	-1902.029	424.166
1000	251.600	426.600	270.900	155.700	-2408.896	-1891.683	413.422

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 180.763 + 84.984\times10^{-3}T - 38.491\times10^{5}T^{-2}$
$H° - H°_{298} = 180.763\times10^{-3}T + 42.492\times10^{-6}T^{2} + 38.491\times10^{2}T^{-1} - 70.582$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -2442.187 + 35.229\times10^{-3}T - 1.893\times10^{-6}T^{2} + 3772.079T^{-1}$
$\Delta Gf° = -2442.187 - 35.229\times10^{-3}T\ln T + 1.893\times10^{-6}T^{2} + 1886.040T^{-1} + 789.822\times10^{-3}T$
922-933.61 K: $\Delta Hf° = -2444.200 + 33.912\times10^{-3}T - 1.416\times10^{-6}T^{2} + 3374.060T^{-1}$
$\Delta Gf° = -2444.200 - 33.912\times10^{-3}T\ln T + 1.416\times10^{-6}T^{2} + 1687.030T^{-1} + 783.689\times10^{-3}T$
933.61-980 K: $\Delta Hf° = -2444.306 + 33.661\times10^{-3}T - 1.271\times10^{-6}T^{2} + 3372.603T^{-1}$
$\Delta Gf° = -2444.306 - 33.661\times10^{-3}T\ln T + 1.271\times10^{-6}T^{2} + 1686.302T^{-1} + 782.222\times10^{-3}T$
980-1000 K: $\Delta Hf° = -2444.271 + 33.481\times10^{-3}T - 1.177\times10^{-6}T^{2} + 3379.764T^{-1}$
$\Delta Gf° = -2444.271 - 33.481\times10^{-3}T\ln T + 1.177\times10^{-6}T^{2} + 1689.882T^{-1} + 781.036\times10^{-3}T$

Source: Data from Bennington (34).

$Fe_2N(c)$
Diiron Nitride
[Formation: $2Fe(c) + 0.5N_2(g) = Fe_2N(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.700	24.200	24.200	0	-.900	2.596	-1.903
300	16.740	24.300	24.200	.030	-.899	2.618	-1.907
400	17.350	29.200	24.850	1.740	-.789	3.778	-2.064
500	17.960	33.140	26.140	3.500	-.744	4.905	-2.144
600	18.560	36.460	27.577	5.330	-.745	6.044	-2.201
700	19.170	39.370	29.070	7.210	-.819	7.172	-2.239
800	19.780	41.970	30.520	9.160	-.970	8.324	-2.274
900	20.390	44.340	31.929	11.170	-1.263	9.499	-2.307
1000	21.000	46.520	33.280	13.240	-1.853	10.721	-2.343

*Data except enthalpy of formation and entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 14.910 + 6.090\text{x}10^{-3}T$
$H°-H°_{298} = 14.910\text{x}10^{-3}T + 3.045\text{x}10^{-6}T^2 - 4.716$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -5.217 + 12.093\text{x}10^{-3}T - 9.391\text{x}10^{-6}T^2 + 460.950T^{-1}$
$\Delta Gf° = -5.217 - 12.093\text{x}10^{-3}T\ln T + 9.391\text{x}10^{-6}T^2 + 230.475T^{-1} + 89.715\text{x}10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Rossini (431). Other data are those estimated by Kelley (243).

$Fe_4N(c)$
Tetrairon Nitride
[Formation: $4Fe(c) + 0.5N_2(g) = Fe_4N(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	29.300	37.000	37.000	0	-2.500	1.067	-.782
300	29.300	37.180	37.013	.050	-2.500	1.086	-.791
400	30.100	45.720	38.170	3.020	-2.383	2.259	-1.234
500	30.900	52.520	40.360	6.080	-2.403	3.430	-1.499
600	31.700	58.230	42.880	9.210	-2.577	4.609	-1.679
700	32.600	63.190	45.447	12.420	-2.911	5.823	-1.818
800	33.400	67.590	47.940	15.720	-3.442	7.106	-1.941
900	34.200	71.560	50.338	19.100	-4.289	8.482	-2.060
1000	35.000	75.210	52.650	22.560	-5.761	9.963	-2.177

*Data except enthalpy of formation and entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 26.840 + 8.160\times10^{-3}T$

$H°- H°_{298} = 26.840\times10^{-3}T + 4.080\times10^{-6}T^2 - 8.365$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -11.051 + 24.465\times10^{-3}T - 20.498\times10^{-6}T^2 + 917.950T^{-1}$

$\Delta Gf° = -11.051 - 24.465\times10^{-3}T\ln T + 20.498\times10^{-6}T^2 + 458.975T^{-1} + 168.765\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (514). Other data are those estimated by Kelley (243).

$(Na_{1.9}Ca_{0.1})(Fe^{+3}_{2.024}Fe^{+2}_{2.501}Mg_{0.475})(Si_{7.971}Al_{0.029}O_{22.095})(OH)_{1.905}(c)$

Crocidolite

[Formation: $1.9Na(c,l) + 0.1Ca(c) + 4.525Fe(c) + 0.475Mg(c,l) + 7.971Si(c) + 0.029Al(c,l)$
$+ 12O_2(g) + 0.9525H_2(g) =$ Crocidolite(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	161.700	161.100	161.100	0	-2433.560	-2269.481	1663.553
300	162.300	162.100	161.100	.300	-2433.579	-2268.458	1652.550
371	179.127	198.460	164.833	12.476	-2433.931	-2229.346	1313.253
371	179.127	198.460	164.833	12.476	-2435.113	-2229.346	1313.253
400	186.000	212.200	167.775	17.770	-2435.087	-2213.262	1209.255
500	204.000	255.700	181.080	37.310	-2434.217	-2157.857	943.186
600	217.000	294.100	196.783	58.390	-2432.531	-2102.741	765.913
700	225.900	328.300	213.214	80.560	-2430.438	-2047.970	639.397
720	227.020	334.680	216.500	85.089	-2430.005	-2037.049	618.321
720	227.020	334.680	216.500	85.089	-2430.027	-2037.049	618.321
800	231.500	358.800	229.425	103.500	-2428.264	-1993.382	544.560
900	234.800	386.300	245.411	126.800	-2426.475	-1939.180	470.891
922	235.196	391.975	248.841	131.970	-2426.167	-1927.274	456.833
922	235.196	391.975	248.841	131.970	-2427.183	-1927.274	456.833
933.61	235.405	394.920	250.639	134.702	-2427.046	-1920.979	449.678
933.61	235.405	394.920	250.639	134.702	-2427.121	-1920.979	449.678
1000	236.600	411.200	260.800	150.400	-2426.518	-1884.993	411.960
1043	237.159	421.173	267.208	160.586	-2426.766	-1861.706	390.096
1100	237.900	433.800	275.527	174.100	-2426.509	-1830.898	363.761

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 191.906 + 54.980\times10^{-3}T - 41.423\times10^{5}T^{-2}$
$H°-H°_{298} = 191.906\times10^{-3}T + 27.490\times10^{-6}T^2 + 41.423\times10^{2}T^{-1} - 73.554$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -2458.046 + 44.263\times10^{-3}T - 19.031\times10^{-6}T^2 + 3870.137T^{-1}$
$\Delta Gf° = -2458.046 - 44.263\times10^{-3}T\ln T + 19.031\times10^{-6}T^2 + 1935.069T^{-1} + 857.202\times10^{-3}T$

371-720 K: $\Delta Hf° = -2458.783 + 38.463\times10^{-3}T - 10.006\times10^{-6}T^2 + 4042.847T^{-1}$
$\Delta Gf° = -2458.783 - 38.463\times10^{-3}T\ln T + 10.006\times10^{-6}T^2 + 2021.424T^{-1} + 827.593\times10^{-3}T$

720-922 K: $\Delta Hf° = -2458.958 + 38.856\times10^{-3}T - 10.243\times10^{-6}T^2 + 4036.747T^{-1}$
$\Delta Gf° = -2458.958 - 38.856\times10^{-3}T\ln T + 10.243\times10^{-6}T^2 + 2018.374T^{-1} + 830.260\times10^{-3}T$

922-933.61 K: $\Delta Hf° = -2459.586 + 38.445\times10^{-3}T - 10.094\times10^{-6}T^2 + 3912.440T^{-1}$
$\Delta Gf° = -2459.586 - 38.445\times10^{-3}T\ln T + 10.094\times10^{-6}T^2 + 1956.220T^{-1} + 828.345\times10^{-3}T$

933.61-1043 K: $\Delta Hf° = -2459.623 + 38.358\times10^{-3}T - 10.044\times10^{-6}T^2 + 3911.935T^{-1}$
$\Delta Gf° = -2459.623 - 38.358\times10^{-3}T\ln T + 10.044\times10^{-6}T^2 + 1955.968T^{-1} + 827.837\times10^{-3}T$

1043-1100 K: $\Delta Hf° = -2353.010 - 160.656\times10^{-3}T + 83.674\times10^{-6}T^2 + 2877.973T^{-1}$
$\Delta Gf° = -2353.010 + 160.656\times10^{-3}T\ln T - 83.674\times10^{-6}T^2 + 1438.986T^{-1} - 559.278\times10^{-3}T$

Source: Data from Bennington (34).

$FeO(g)$
Iron Monoxide (ideal gas)
[Formation: $Fe(c,l) + 0.5O_2(g) = FeO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$C_p°$	$S°$	$-(G° - H°_{298})/T$	$H° - H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	7.510	56.007	56.007	0	65.500	58.051	-42.552
300	7.520	56.054	56.007	.014	65.496	58.005	-42.256
400	7.890	58.268	56.306	.785	65.287	55.539	-30.345
500	8.180	60.062	56.884	1.589	65.043	53.129	-23.222
600	8.380	61.573	57.543	2.418	64.757	50.772	-18.494
700	8.520	62.876	58.213	3.264	64.420	48.469	-15.132
800	8.620	64.021	58.870	4.121	64.013	46.215	-12.625
900	8.700	65.041	59.500	4.987	63.509	44.020	-10.689
1000	8.750	65.960	60.100	5.860	62.833	41.888	-9.154
1043	8.771	66.329	60.349	6.237	62.396	40.996	-8.590
1100	8.800	66.797	60.672	6.738	61.959	39.840	-7.915
1185	8.834	67.453	61.134	7.487	61.465	38.149	-7.036
1185	8.834	67.453	61.134	7.487	61.250	38.149	-7.036
1200	8.840	67.564	61.214	7.620	61.197	37.857	-6.895
1300	8.870	68.273	61.731	8.505	60.833	35.926	-6.040
1400	8.900	68.932	62.222	9.394	60.449	34.024	-5.311
1500	8.920	69.546	62.689	10.285	60.045	32.151	-4.684
1600	8.940	70.123	63.137	11.178	59.618	30.305	-4.139
1667	8.953	70.489	63.424	11.777	59.320	29.084	-3.813
1667	8.953	70.489	63.424	11.777	59.120	29.084	-3.813
1700	8.960	70.665	63.563	12.073	58.945	28.491	-3.663
1800	8.980	71.178	63.972	12.970	58.398	26.716	-3.244
1811	8.981	71.233	64.016	13.069	58.333	26.520	-3.200
1811	8.981	71.233	64.016	13.069	55.033	26.520	-3.200
1900	8.990	71.664	64.365	13.868	54.455	25.131	-2.891
2000	9.010	72.125	64.741	14.768	53.805	23.605	-2.579
2100	9.020	72.565	65.104	15.669	53.154	22.110	-2.301
2200	9.030	72.985	65.452	16.572	52.502	20.647	-2.051
2300	9.040	73.387	65.789	17.476	51.848	19.213	-1.826
2400	9.050	73.772	66.113	18.381	51.193	17.809	-1.622
2500	9.070	74.142	66.427	19.287	50.535	16.431	-1.436

Phase changes:
1043 K, Curie temperature of Fe; $\Delta H° = 0$ kcal/mol.
1185 K, $\alpha - \gamma$ transition point of Fe; $\Delta H° = 0.215$ kcal/mol.
1667 K, $\gamma - \delta$ transition point of Fe; $\Delta H° = 0.200$ kcal/mol.
1811 K, melting point of Fe; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $C_p° = 8.445 + 0.328\times10^{-3}T - 0.918\times10^{5}T^{-2}$
$H° - H°_{298} = 8.445\times10^{-3}T + 0.164\times10^{-6}T^2 + 0.918\times10^{2}T^{-1} - 2.840$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf° = 63.543 + 5.051\times10^{-3}T - 6.158\times10^{-6}T^2 + 297.700T^{-1}$
$\Delta Gf° = 63.543 - 5.051\times10^{-3}T\ln T + 6.158\times10^{-6}T^2 + 148.850T^{-1} + 6.847\times10^{-3}T$
1043-1185 K: $\Delta Hf° = 87.104 - 38.930\times10^{-3}T + 14.552\times10^{-6}T^2 + 69.200T^{-1}$
$\Delta Gf° = 87.104 + 38.930\times10^{-3}T\ln T - 14.552\times10^{-6}T^2 + 34.600T^{-1} - 299.697\times10^{-3}T$
1185-1667 K: $\Delta Hf° = 63.490 - 0.675\times10^{-3}T - 1.138\times10^{-6}T^2 + 188.200T^{-1}$
$\Delta Gf° = 63.490 + 0.675\times10^{-3}T\ln T + 1.138\times10^{-6}T^2 + 94.100T^{-1} - 27.656\times10^{-3}T$
1667-1811 K: $\Delta Hf° = -19.405 + 47.822\times10^{-3}T - 10.769\times10^{-6}T^2 + 47887.400T^{-1}$
$\Delta Gf° = -19.405 - 47.822\times10^{-3}T\ln T + 10.769\times10^{-6}T^2 + 23943.700T^{-1} + 357.222\times10^{-3}T$
1811-2000 K: $\Delta Hf° = 66.445 - 6.170\times10^{-3}T - 0.087\times10^{-6}T^2 + 69.200T^{-1}$
$\Delta Gf° = 66.445 + 6.170\times10^{-3}T\ln T + 0.087\times10^{-6}T^2 + 34.600T^{-1} - 68.576\times10^{-3}T$
2000-2500 K: $\Delta Hf° = 67.113 - 6.725\times10^{-3}T + 0.059\times10^{-6}T^2 - 223.200T^{-1}$
$\Delta Gf° = 67.113 + 6.725\times10^{-3}T\ln T - 0.059\times10^{-6}T^2 - 111.600T^{-1} - 72.798\times10^{-3}T$

Source: Data from Pedley (396).

$FeOCl(c)$
Iron Oxychloride
[Formation: $Fe(c) + 0.5O_2(g) + 0.5Cl_2(g) = FeOCl(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	16.850	19.730	19.730	0	-98.230	-86.919	63.712
300	16.870	19.840	19.737	.031	-98.224	-86.851	63.270
400	18.100	24.880	20.417	1.785	-97.866	-83.113	45.410
500	19.000	29.020	21.738	3.641	-97.484	-79.470	34.736
600	19.900	32.560	23.250	5.586	-97.088	-75.901	27.647
700	20.950	35.700	24.806	7.626	-96.671	-72.401	22.604

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 16.021 + 6.940 \times 10^{-3}T - 1.104 \times 10^{5}T^{-2}$
$H°-H°_{298} = 16.021 \times 10^{-3}T + 3.470 \times 10^{-6}T^{2} + 1.104 \times 10^{2}T^{-1} - 5.455$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -101.368 + 8.214 \times 10^{-3}T - 2.896 \times 10^{-6}T^{2} + 282.150T^{-1}$
$\Delta Gf° = -101.368 - 8.214 \times 10^{-3}T\ln T + 2.896 \times 10^{-6}T^{2} + 141.075T^{-1} + 92.808 \times 10^{-3}T$

Source: Data from Stuve (483).

$FeSO_4(c)$
Iron Sulfate
[Reaction: $Fe(c,l) + 0.5S_2(g) + 2O_2(g) = FeSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	24.040	28.909	28.909	0	-238.155	-207.483	152.087
300	24.140	29.058	28.090	.045	-238.154	-207.292	151.010
400	27.880	36.535	29.905	2.652	-237.992	-197.023	107.647
500	30.810	43.085	31.899	5.593	-237.609	-186.821	81.658
600	32.990	48.904	34.257	8.788	-237.085	-176.710	64.366
700	34.570	54.113	36.727	12.170	-236.484	-166.693	52.043
800	35.710	58.808	39.199	15.687	-235.864	-156.768	42.826
900	36.510	63.061	41.618	19.299	-235.282	-146.916	35.676
1000	37.160	66.943	43.960	22.983	-234.831	-137.126	29.968
1043	37.396	68.512	44.940	24.586	-234.773	-132.926	27.853
1100	37.710	70.511	46.214	26.727	-234.544	-127.364	25.305
1185	38.126	73.333	48.058	29.951	-234.029	-119.100	21.965
1185	38.126	73.333	48.058	29.951	-234.244	-119.100	21.965
1200	38.200	73.813	48.377	30.523	-234.117	-117.644	21.426
1300	38.640	76.889	50.454	34.365	-233.261	-107.974	18.152
1400	39.040	79.767	52.446	38.250	-232.404	-98.367	15.356
1500	39.420	82.473	54.358	42.173	-231.544	-88.824	12.941
1600	39.780	85.029	56.196	46.133	-230.684	-79.337	10.837
1667	40.008	86.666	57.388	48.806	-230.108	-73.011	9.572
1667	40.008	86.666	57.388	48.806	-230.308	-73.011	9.572
1700	40.120	87.451	57.964	50.128	-230.050	-69.900	8.986
1800	40.460	89.754	59.667	54.157	-229.269	-60.500	7.346
1811	40.495	90.001	59.850	54.602	-229.186	-59.472	7.177
1811	40.495	90.001	59.850	54.602	-232.486	-59.472	7.177
1900	40.780	91.950	61.308	58.219	-231.864	-50.985	5.865
2000	41.100	94.050	62.894	62.313	-231.146	-41.484	4.533

Phase changes:
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 32.560 + 4.868\times10^{-3}T - 8.864\times10^{5}T^{-2}$
$H°- H°_{298} = 32.560\times10^{-3}T + 2.434\times10^{-6}T^{2} + 8.864\times10^{2}T^{-1} - 12.897$

Reaction equations (kcal/mol):

298.15-1043 K: $\Delta Hr° = -245.268 + 14.150\times10^{-3}T - 4.803\times10^{-6}T^{2} + 990.350T^{-1}$
$\Delta Gr° = -245.268 - 14.150\times10^{-3}T\ln T + 4.803\times10^{-6}T^{2} + 495.175T^{-1} + 200.348\times10^{-3}T$
1043-1185 K: $\Delta Hr° = -221.708 - 29.831\times10^{-3}T + 15.908\times10^{-6}T^{2} + 761.850T^{-1}$
$\Delta Gr° = -221.708 + 29.831\times10^{-3}T\ln T - 15.908\times10^{-6}T^{2} + 380.925T^{-1} - 106.196\times10^{-3}T$
1185-1667 K: $\Delta Hr° = -245.321 + 8.424\times10^{-3}T + 0.217\times10^{-6}T^{2} + 880.850T^{-1}$
$\Delta Gr° = -245.321 - 8.424\times10^{-3}T\ln T - 0.217\times10^{-6}T^{2} + 440.425T^{-1} + 165.844\times10^{-3}T$
1667-1811 K: $\Delta Hr° = -328.216 + 56.921\times10^{-3}T - 9.414\times10^{-6}T^{2} + 48580.050T^{-1}$
$\Delta Gr° = -328.216 - 56.921\times10^{-3}T\ln T + 9.414\times10^{-6}T^{2} + 24290.025T^{-1} + 550.723\times10^{-3}T$
1811-2000 K: $\Delta Hr° = -242.366 + 2.929\times10^{-3}T + 1.268\times10^{-6}T^{2} + 761.850T^{-1}$
$\Delta Gr° = -242.366 - 2.929\times10^{-3}T\ln T - 1.268\times10^{-6}T^{2} + 380.925T^{-1} + 124.925\times10^{-3}T$

Source: Data from DeKock (112).

$Fe_2(SO_4)_3(c)$
Diiron Sulfate
[Reaction: $2Fe(c) + 1.5S_2(g) + 6O_2(g) = Fe_2(SO_4)_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	64.950	67.550	67.550	0	-663.165	-567.376	415.892
300	65.207	67.953	67.553	.120	-663.166	-566.780	412.893
400	76.317	88.369	70.262	7.243	-662.752	-534.693	292.139
500	84.277	106.287	75.711	15.288	-661.697	-502.787	219.765
600	90.928	122.255	82.162	24.056	-660.206	-471.138	171.610
700	96.850	136.724	88.938	33.450	-658.361	-439.766	137.299
800	102.282	150.015	95.753	43.410	-656.226	-408.687	111.647
800	102.720	150.643	95.753	43.912	-655.724	-408.687	111.647
900	102.720	162.742	102.538	54.184	-653.579	-377.939	91.775

Phase change: 800 K, α - β transition point of $Fe_2(SO_4)_3$; ΔH° = 0.502 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp^\circ = 64.094 + 50.432\times10^{-3}T - 12.605\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 64.094\times10^{-3}T + 25.216\times10^{-6}T^2 + 12.605\times10^{2}T^{-1} - 25.579$
800-900 K: $Cp^\circ = 102.720$
$H^\circ - H^\circ_{298} = 102.720\times10^{-3}T - 38.264$

Reaction equations (kcal/mol):

298.15-800 K: $\Delta Hr^\circ = -671.100 + 8.642\times10^{-3}T + 9.576\times10^{-6}T^2 + 1343.850T^{-1}$
$\Delta Gr^\circ = -671.100 - 8.642\times10^{-3}T\ln T - 9.576\times10^{-6}T^2 + 671.925T^{-1} + 392.425\times10^{-3}T$
800-900 K: $\Delta Hr^\circ = -683.785 + 47.268\times10^{-3}T - 15.640\times10^{-6}T^2 + 83.350T^{-1}$
$\Delta Gr^\circ = -683.785 - 47.268\times10^{-3}T\ln T + 15.640\times10^{-6}T^2 + 41.675T^{-1} + 647.293\times10^{-3}T$

Source: Data from DeKock (112).

$FeSO_4 \cdot H_2O(c)$
Iron Sulfate Monohydrate
[Reaction: $Fe(c) + 0.5S_2(g) + 2.5O_2(g) + H_2(g) = FeSO_4 \cdot H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	33.346	37.700	37.700	0	-312.755	-268.094	196.516
300	33.513	37.907	37.700	.062	-312.756	-267.816	195.102
350	38.015	43.411	38.125	1.850	-312.699	-260.329	162.555
400	42.517	48.781	39.123	3.863	-312.449	-252.862	138.156
450	47.019	54.049	40.489	6.102	-312.005	-245.438	119.199
500	51.521	59.236	42.106	8.565	-311.370	-238.074	104.061
550	56.023	64.357	43.895	11.254	-310.539	-230.782	91.703

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 6.509 + 90.016\times10^{-3}T - 0.001\times10^{5}T^{-2}$

$H° - H°_{298} = 6.509\times10^{-3}T + 45.008\times10^{-6}T^{2} + 0.001\times10^{2}T^{-1} - 5.942$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -309.830 - 21.973\times10^{-3}T + 37.101\times10^{-6}T^{2} + 97.950T^{-1}$

$\Delta Gr° = -309.830 + 21.973\times10^{-3}T\ln T - 37.101\times10^{-6}T^{2} + 48.975T^{-1} + 25.304\times10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$FeSO_4 \cdot 4H_2O(c)$
Iron Sulfate Tetrahydrate
[Reaction: $Fe(c) + 0.5S_2(g) + 4O_2(g) + 4H_2(g) = FeSO_4 \cdot 4H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	65.924	67.500	67.500	0	-524.855	-439.250	321.975
300	66.190	67.909	67.502	.122	-524.855	-438.719	319.602
350	73.390	78.653	68.333	3.612	-524.663	-424.373	264.987
400	80.590	88.922	70.270	7.461	-524.157	-410.076	224.052
450	87.790	98.830	72.894	11.671	-523.334	-395.862	192.254
500	94.990	108.452	75.972	16.240	-522.193	-381.756	166.863
550	102.190	117.844	79.353	21.170	-520.733	-367.781	146.141

*Data except enthalpy of formation and entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 23.150 + 143.600 \times 10^{-3}T$

$H° - H°_{298} = 23.150 \times 10^{-3}T + 71.800 \times 10^{-6}T^2 - 13.285$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -520.025 - 35.545 \times 10^{-3}T + 61.881 \times 10^{-6}T^2 + 79.550T^{-1}$

$\Delta Gr° = -520.025 + 35.545 \times 10^{-3}T\ln T - 61.881 \times 10^{-6}T^2 + 39.775T^{-1} + 86.405 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation and entropy at 298 K.

$FeSO_4 \cdot 7H_2O(c)$
Iron Sulfate Heptahydrate
[Reaction: $Fe(c) + 0.5S_2(g) + 5.5O_2(g) + 7H_2(g) = FeSO_4 \cdot 7H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	94.313	97.800	97.800	0	-735.795	-609.394	446.692
300*	94.784	98.385	97.802	.175	-735.801	-608.610	443.366
350	107.210	113.937	99.003	5.227	-735.614	-587.418	366.796
400	119.049	129.032	101.817	10.886	-734.878	-566.290	309.403
450	130.300	143.709	105.660	17.122	-733.621	-545.288	264.824
500	140.964	157.995	110.183	23.906	-731.867	-524.451	229.234
550	151.040	171.907	115.163	31.209	-729.644	-503.813	200.194

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp^\circ = 42.126 + 203.858\times10^{-3}T - 7.639\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 42.126\times10^{-3}T + 101.929\times10^{-6}T^{2} + 7.639\times10^{2}T^{-1} - 24.183$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr^\circ = -732.615 - 46.781\times10^{-3}T + 89.999\times10^{-6}T^{2} + 825.150T^{-1}$
$\Delta Gr^\circ = -732.615 + 46.781\times10^{-3}T\ln T - 89.999\times10^{-6}T^{2} + 412.575T^{-1} + 168.933\times10^{-3}T$

Source: Data from DeKock (112) who estimated all above 298 K.

$FeSb_2(c,l)$
Iron Diantimonide
[Formation: $Fe(c) + 2Sb(c,l) = FeSb_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°₂₉₈)/T	H°- H°₂₉₈	ΔHf°	ΔGf°	
298.15	19.080	25.980	25.980	0	-7.080	-6.394	4.687
300	19.090	26.100	25.983	.035	-7.078	-6.389	4.654
400	19.580	31.660	26.737	1.969	-6.994	-6.172	3.372
500	19.960	36.070	28.178	3.946	-6.953	-5.971	2.610
600	20.450	39.740	29.800	5.964	-6.952	-5.778	2.105
700	21.210	42.950	31.459	8.044	-6.985	-5.577	1.741
800	22.120	45.840	33.077	10.210	-7.056	-5.381	1.470
900	23.110	48.500	34.644	12.470	-7.198	-5.159	1.253
903.9	23.176	48.600	34.704	12.560	-7.206	-5.150	1.245
903.9	23.176	48.600	34.704	12.560	-16.706	-5.150	1.245
1000	24.800	51.010	36.155	14.855	-16.947	-3.917	.856
1021.2	25.410	51.540	36.473	15.385	-17.046	-3.644	.780
1021.2	33.590	64.180	36.473	28.295	-4.136	-3.644	.780
1030	33.590	64.470	36.718	28.585	-4.055	-3.647	.774

Phase changes: 903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.
1021.2 K, peritectic decomposition point of $FeSb_2$; ΔH° = 12.190 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1021.2 K: $Cp° = 14.775 + 9.162\times10^{-3}T + 1.397\times10^{5}T^{-2}$
$H° - H°_{298} = 14.775\times10^{-3}T + 4.581\times10^{-6}T^{2} - 1.397\times10^{2}T^{-1} - 4.344$
1021.2-1030 K: $Cp° = 33.590$
$H° - H°_{298} = 33.590\times10^{-3}T - 6.007$

Formation equations (kcal/mol):

298.15-903.9 K: $\Delta Hf° = -8.619 + 4.820\times10^{-3}T - 3.834\times10^{-6}T^{2} + 132.000T^{-1}$
$\Delta Gf° = -8.619 - 4.820\times10^{-3}T\ln T + 3.834\times10^{-6}T^{2} + 66.000T^{-1} + 33.039\times10^{-3}T$
903.9-1021.2 K: $\Delta Hf° = -15.626 - 0.004\times10^{-3}T - 1.490\times10^{-6}T^{2} + 88.800T^{-1}$
$\Delta Gf° = -15.626 + 0.004\times10^{-3}T\ln T + 1.490\times10^{-6}T^{2} + 44.400T^{-1} + 10.100\times10^{-3}T$
1021.2-1030 K: $\Delta Hf° = -17.289 + 18.811\times10^{-3}T - 6.071\times10^{-6}T^{2} + 228.500T^{-1}$
$\Delta Gf° = -17.289 - 18.811\times10^{-3}T\ln T + 6.071\times10^{-6}T^{2} + 114.250T^{-1} + 137.348\times10^{-3}T$

Source: Data from Gronvold (188).

$FeSe_{0.961}(c)$

Iron Selenide

[Reaction: $Fe(c) + 0.4805Se_2(g) = FeSe_{0.961}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	13.090	16.540	16.540	0	-32.001	-26.650	19.535
300	13.120	16.620	16.540	.024	-31.996	-26.617	19.390
400	14.220	20.570	17.077	1.397	-31.727	-24.867	13.586
500	15.010	23.830	18.110	2.860	-31.431	-23.185	10.134
600	15.670	26.620	19.295	4.395	-31.119	-21.561	7.853
700	16.260	29.080	20.520	5.992	-30.802	-19.991	6.241
730.8	16.440	29.790	20.900	6.495	-30.707	-19.521	5.838
730.8	14.110	32.920	20.900	8.786	-28.416	-19.521	5.838
800	13.910	34.190	21.996	9.755	-28.388	-18.680	5.103
900	14.540	35.850	23.440	11.169	-28.419	-17.461	4.240
1000	16.020	37.460	24.769	12.691	-28.513	-16.249	3.551

Phase change: 730.8 K, α - β transition point of $FeSe_{0.961}$; ΔH° = 2.291 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-730.8 K: $Cp° = 13.046 + 4.960\times10^{-3}T - 1.275\times10^{5}T^{-2}$
$H° - H°_{298} = 13.046\times10^{-3}T + 2.480\times10^{-6}T^{2} + 1.275\times10^{2}T^{-1} - 4.538$
730.8-1000 K: $Cp° = -24.039 + 32.190\times10^{-3}T + 78.104\times10^{5}T^{-2}$
$H° - H°_{298} = -24.039\times10^{-3}T + 16.095\times10^{-6}T^{2} - 78.104\times10^{2}T^{-1} + 28.445$

Reaction equations (kcal/mol):

298.15-730.8 K: $\Delta Hr° = -35.220 + 8.143\times10^{-3}T - 3.438\times10^{-6}T^{2} + 327.218T^{-1}$
$\Delta Gr° = -35.220 - 8.143\times10^{-3}T\ln T + 3.438\times10^{-6}T^{2} + 163.609T^{-1} + 72.274\times10^{-3}T$
730.8-1000 K: $\Delta Hr° = -2.237 - 28.942\times10^{-3}T + 10.177\times10^{-6}T^{2} - 7610.682T^{-1}$
$\Delta Gr° = -2.237 + 28.942\times10^{-3}T\ln T - 10.177\times10^{-6}T^{2} - 3805.341T^{-1} - 200.022\times10^{-3}T$

Source: Data from Mills (332).

$FeSe_{1.143}(c)$

Iron Selenide

[Reaction: $Fe(c) + 0.5715Se_2(g) = FeSe_{1.143}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	15.140	20.950	20.950	0	-34.831	-29.216	21.416
300	15.180	21.040	20.950	.028	-34.824	-29.180	21.258
400	18.180	25.710	21.570	1.656	-34.391	-27.361	14.949
451	21.030	28.050	22.165	2.654	-34.027	-26.484	12.834
451	17.150	28.050	22.165	2.654	-34.027	-26.484	12.834
500	15.840	29.740	22.830	3.455	-33.850	-25.675	11.223
600	17.090	32.680	24.233	5.068	-33.552	-24.070	8.767
638	29.690	34.110	24.773	5.957	-33.178	-23.476	8.042
638	15.860	34.110	24.773	5.957	-33.178	-23.476	8.042
700	15.760	35.580	25.670	6.937	-33.055	-22.541	7.038
800	15.700	37.670	27.036	8.507	-32.926	-21.042	5.748
900	16.010	39.540	28.329	10.090	-32.879	-19.567	4.751
1000	16.550	41.250	29.534	11.716	-32.960	-18.085	3.952

Phase change: 451 K, second order transition point of $FeSe_{1.143}$; ΔH° = 0 kcal/mol.
638 K, second order transition point of $FeSe_{1.143}$; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-451 K: $Cp^\circ = -22.758 + 84.900\text{x}10^{-3}T + 11.187\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = -22.758\text{x}10^{-3}T + 42.450\text{x}10^{-6}T^2 - 11.187\text{x}10^{2}T^{-1} + 6.764$
451-638 K: $Cp^\circ = -15.054 + 47.182\text{x}10^{-3}T + 20.218\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = -15.054\text{x}10^{-3}T + 23.591\text{x}10^{-6}T^2 - 20.218\text{x}10^{2}T^{-1} + 9.128$
638-1000 K: $Cp^\circ = 6.264 + 8.552\text{x}10^{-3}T + 16.854\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 6.264\text{x}10^{-3}T + 4.276\text{x}10^{-6}T^2 - 16.854\text{x}10^{2}T^{-1} + 2.862$

Reaction equations (kcal/mol):

298.15-451 K: $\Delta Hr^\circ = -26.444 - 28.631\text{x}10^{-3}T + 36.561\text{x}10^{-6}T^2 - 924.433T^{-1}$
$\Delta Gr^\circ = -26.444 + 28.631\text{x}10^{-3}T\ln T - 36.561\text{x}10^{-6}T^2 - 462.216T^{-1} - 156.329\text{x}10^{-3}T$
451-638 K: $\Delta Hr^\circ = -24.080 - 20.927\text{x}10^{-3}T + 17.702\text{x}10^{-6}T^2 - 1827.533T^{-1}$
$\Delta Gr^\circ = -24.080 + 20.927\text{x}10^{-3}T\ln T - 17.702\text{x}10^{-6}T^2 - 913.766T^{-1} - 120.773\text{x}10^{-3}T$
638-1000 K: $\Delta Hr^\circ = -30.346 + 0.391\text{x}10^{-3}T - 1.613\text{x}10^{-6}T^2 - 1491.133T^{-1}$
$\Delta Gr^\circ = -30.346 - 0.391\text{x}10^{-3}T\ln T + 1.613\text{x}10^{-6}T^2 - 745.566T^{-1} + 13.991\text{x}10^{-3}T$

Source: Data from Mills (332).

$FeSe_{1.333}(c)$

Iron Selenide
[Reaction: $Fe(c) + 0.6667Se_2(g) = FeSe_{1.333}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	17.530	22.290	22.290	0	-39.101	-32.234	23.628
300	17.610	22.400	22.297	.031	-39.093	-32.193	23.453
307	17.850	22.820	22.302	.159	-39.053	-32.032	22.803
307	16.060	22.820	22.302	.159	-39.053	-32.032	22.803
400	16.320	27.090	22.933	1.663	-38.750	-29.945	16.361
500	16.730	30.780	24.152	3.314	-38.454	-27.783	12.144
600	17.210	33.870	25.518	5.011	-38.168	-25.675	9.352
700	17.720	36.560	26.907	6.757	-37.890	-23.612	7.372
800	19.000	38.990	28.265	8.580	-37.604	-21.588	5.898
900	21.430	41.360	29.589	10.594	-37.221	-19.610	4.762
978	60.950	43.730	30.613	12.828	-36.365	-18.112	4.047
978	20.400	43.730	30.613	12.828	-36.365	-18.112	4.047
1000	20.690	44.180	30.900	13.280	-36.337	-17.695	3.867
1043	21.262	45.063	31.466	14.182	-36.355	-16.894	3.540
1100	22.020	46.220	32.205	15.416	-36.196	-15.836	3.146

Phase changes: 307 K, second order transition point of $FeSe_{1.333}$; ΔH° = 0 kcal/mol.
978 K, second order transition point of $FeSe_{1.333}$; ΔH° = 0 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-307 K: $Cp° = -11.854 + 98.554\times10^{-3}T$
$H°-H°_{298} = -11.854\times10^{-3}T + 49.277\times10^{-6}T^2 - 0.846$
307-978 K: $Cp° = 4.060 + 20.240\times10^{-3}T + 5.453\times10^{5}T^{-2}$
$H°-H°_{298} = 4.060\times10^{-3}T + 10.120\times10^{-6}T^2 - 5.453\times10^{2}T^{-1} - 0.265$
978-1100 K: $Cp° = 5.735 + 14.396\times10^{-3}T + 5.609\times10^{5}T^{-2}$
$H°-H°_{298} = 5.735\times10^{-3}T + 7.198\times10^{-6}T^2 - 5.609\times10^{2}T^{-1} + 0.908$

Reaction equations (kcal/mol):

298.15-307 K: $\Delta Hr° = -38.005 - 18.743\times10^{-3}T + 43.419\times10^{-6}T^2 + 188.565T^{-1}$
$\Delta Gr° = -38.005 + 18.743\times10^{-3}T\ln T - 43.419\times10^{-6}T^2 + 94.282T^{-1} - 75.548\times10^{-3}T$
307-978 K: $\Delta Hr° = -37.424 - 2.829\times10^{-3}T + 4.262\times10^{-6}T^2 - 356.735T^{-1}$
$\Delta Gr° = -37.424 + 2.829\times10^{-3}T\ln T - 4.262\times10^{-6}T^2 - 178.368T^{-1} + 4.568\times10^{-3}T$
978-1043 K: $\Delta Hr° = -36.251 - 1.154\times10^{-3}T + 1.340\times10^{-6}T^2 - 372.335T^{-1}$
$\Delta Gr° = -36.251 + 1.154\times10^{-3}T\ln T - 1.340\times10^{-6}T^2 - 186.168T^{-1} + 12.053\times10^{-3}T$
1043-1100 K: $\Delta Hr° = -12.690 - 45.135\times10^{-3}T + 22.051\times10^{-6}T^2 - 600.835T^{-1}$
$\Delta Gr° = -12.690 + 45.135\times10^{-3}T\ln T - 22.051\times10^{-6}T^2 - 300.418T^{-1} - 294.492\times10^{-3}T$

Source: Data from Mills (332).

$FeSe_2(c,l)$
Iron Diselenide
[Reaction: $Fe(c) + Se_2(g) = FeSe_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	16.870	19.950	19.950	0	-62.700	-49.352	36.175
300	16.888	20.054	19.951	.031	-62.698	-49.269	35.892
400	17.875	25.046	20.623	1.769	-62.581	-44.810	24.483
500	19.094	29.302	21.932	3.685	-62.355	-40.385	17.652
600	21.439	32.965	23.468	5.698	-62.090	-36.013	13.118
700	27.087	36.625	25.085	8.078	-61.515	-31.705	9.899
800	39.352	40.974	26.788	11.349	-60.117	-27.525	7.519
856.7	47.800	43.949	27.822	13.816	-58.748	-25.261	6.444
856.7	33.700	52.578	27.822	21.208	-51.356	-25.261	6.444
900	32.385	54.221	29.079	22.628	-50.804	-23.980	5.823
1000	44.216	57.861	31.769	26.092	-49.475	-21.066	4.604

Phase change: 856.7 K, peritectic decomposition point of $FeSe_2$; ΔH° = 7.392 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-856.7 K: $Cp^\circ = -16.772 + 62.912\times10^{-3}T + 13.231\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = -16.772\times10^{-3}T + 31.456\times10^{-6}T^{2} - 13.231\times10^{2}T^{-1} + 6.642$
856.7-1000 K: $Cp^\circ = 10.170 + 25.758\times10^{-3}T$
$H^\circ - H^\circ_{298} = 10.170\times10^{-3}T + 12.879\times10^{-6}T^{2} + 3.043$

Reaction equations (kcal/mol):

298.15-856.7 K: $\Delta Hr^\circ = -52.999 - 27.215\times10^{-3}T + 25.704\times10^{-6}T^{2} - 1154.500T^{-1}$
$\Delta Gr^\circ = -52.999 + 27.215\times10^{-3}T\ln T - 25.704\times10^{-6}T^{2} - 577.250T^{-1} - 128.672\times10^{-3}T$
856.7-1000 K: $\Delta Hr^\circ = -56.598 - 0.273\times10^{-3}T + 7.127\times10^{-6}T^{2} + 168.600T^{-1}$
$\Delta Gr^\circ = -56.598 + 0.273\times10^{-3}T\ln T - 7.127\times10^{-6}T^{2} + 84.300T^{-1} + 40.655\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Svendsen (488). Other data from Gronvold (185).

FeSi(c,l)
Iron Silicide
[Formation: $Fe(c) + Si(c,l) = FeSi(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	10.794	10.680	10.680	0	-17.600	-17.499	12.827
300	10.810	10.747	10.680	.020	-17.600	-17.498	12.747
400	11.324	13.926	11.111	1.126	-17.627	-17.464	9.542
500	11.844	16.508	11.940	2.284	-17.697	-17.415	7.612
600	12.364	18.714	12.887	3.496	-17.794	-17.349	6.319
700	12.884	20.660	13.863	4.758	-17.918	-17.266	5.391
800	13.404	22.414	14.824	6.072	-18.074	-17.162	4.688
900	13.924	24.022	15.758	7.438	-18.290	-17.035	4.137
1000	14.444	25.516	16.660	8.856	-18.636	-16.872	3.687
1043	14.668	26.129	17.038	9.482	-18.917	-16.791	3.518
1100	14.964	26.918	17.529	10.328	-19.133	-16.674	3.313
1185	15.406	28.050	18.245	11.618	-19.274	-16.482	3.040
1185	15.406	28.050	18.245	11.618	-19.489	-16.482	3.040
1200	15.484	28.244	18.369	11.850	-19.476	-16.445	2.995
1300	16.004	29.502	19.176	13.424	-19.372	-16.194	2.722
1400	16.524	30.706	19.956	15.050	-19.244	-15.948	2.490
1500	17.044	31.864	20.712	16.728	-19.090	-15.730	2.292
1600	17.564	32.980	21.442	18.460	-18.907	-15.510	2.119
1667	17.913	33.708	21.923	19.647	-18.773	-15.353	2.013
1667	17.913	33.708	21.923	19.647	-18.973	-15.353	2.013
1683	17.996	33.880	22.036	19.934	-18.951	-15.318	1.989
1683	20.000	43.886	22.036	36.774	-2.111	-15.318	1.989
1687	20.000	43.933	22.088	36.854	-2.098	-15.351	1.989
1687	20.000	43.933	22.088	36.854	-14.180	-15.351	1.989
1700	20.000	44.088	22.256	37.114	-14.127	-15.358	1.974
1800	20.000	45.230	23.500	39.114	-13.737	-15.436	1.874

Phase changes:
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1683 K, melting point of FeSi; ΔH° = 16.840 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1683 K: $Cp^\circ = 9.250 + 5.194\times10^{-3}T - 0.004\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 9.250\times10^{-3}T + 2.597\times10^{-6}T^{2} + 0.004\times10^{2}T^{-1} - 2.990$
1683-1800 K: $Cp^\circ = 20.000$
$H^\circ - H^\circ_{298} = 20.000\times10^{-3}T + 3.114$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -18.828 + 3.792\times10^{-3}T - 3.825\times10^{-6}T^{2} + 130.400T^{-1}$
$\Delta Gf^\circ = -18.828 - 3.792\times10^{-3}T\ln T + 3.825\times10^{-6}T^{2} + 65.200T^{-1} + 24.190\times10^{-3}T$
1043-1185 K: $\Delta Hf^\circ = 4.733 - 40.189\times10^{-3}T + 16.886\times10^{-6}T^{2} - 98.100T^{-1}$
$\Delta Gf^\circ = 4.733 + 40.189\times10^{-3}T\ln T - 16.886\times10^{-6}T^{2} - 49.050T^{-1} - 282.355\times10^{-3}T$
1185-1667 K: $\Delta Hf^\circ = -18.881 - 1.934\times10^{-3}T + 1.195\times10^{-6}T^{2} + 20.900T^{-1}$
$\Delta Gf^\circ = -18.881 + 1.934\times10^{-3}T\ln T - 1.195\times10^{-6}T^{2} + 10.450T^{-1} - 10.314\times10^{-3}T$
1667-1683 K: $\Delta Hf^\circ = -101.776 + 46.563\times10^{-3}T - 8.436\times10^{-6}T^{2} + 47720.100T^{-1}$
$\Delta Gf^\circ = -101.776 - 46.563\times10^{-3}T\ln T + 8.436\times10^{-6}T^{2} + 23860.050T^{-1} + 374.565\times10^{-3}T$
1683-1687 K: $\Delta Hf^\circ = -95.672 + 57.313\times10^{-3}T - 11.033\times10^{-6}T^{2} + 47719.700T^{-1}$
$\Delta Gf^\circ = -95.672 - 57.313\times10^{-3}T\ln T + 11.033\times10^{-6}T^{2} + 23859.850T^{-1} + 446.422\times10^{-3}T$
1687-1800 K: $\Delta Hf^\circ = -108.101 + 56.892\times10^{-3}T - 10.682\times10^{-6}T^{2} + 47818.200T^{-1}$
$\Delta Gf^\circ = -108.101 - 56.892\times10^{-3}T\ln T + 10.682\times10^{-6}T^{2} + 23909.100T^{-1} + 451.236\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Other data from Hultgren (210).

$FeSi_2(c)$
Iron Disilicide
[Formation: $Fe(c) + 2Si(c) = FeSi_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	15.330	13.260	13.260	0	-19.400	-18.726	13.726
300	15.360	13.350	13.260	.028	-19.401	-18.721	13.638
400	16.050	17.880	13.890	1.596	-19.473	-18.499	10.107
500	16.740	21.540	15.072	3.234	-19.609	-18.243	7.974
600	17.430	24.630	16.390	4.944	-19.780	-17.940	6.535
700	18.120	27.360	17.756	6.723	-19.978	-17.611	5.498
800	18.840	29.820	19.106	8.571	-20.205	-17.250	4.712
900	19.500	32.070	20.417	10.488	-20.490	-16.858	4.094
1000	20.220	34.170	21.696	12.474	-20.896	-16.426	3.590
1043	20.517	35.028	22.228	13.350	-21.200	-16.228	3.400
1100	20.910	36.120	22.909	14.532	-21.444	-15.952	3.169
1185	21.522	37.709	23.926	16.332	-21.622	-15.536	2.865
1185	21.522	37.709	23.926	16.332	-21.837	-15.536	2.865
1200	21.630	37.980	24.100	16.656	-21.829	-15.457	2.815

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 13.174 + 7.060\times10^{-3}T + 0.046\times10^{5}T^{-2}$
$H°-H°_{298} = 13.174\times10^{-3}T + 3.530\times10^{-6}T^{2} - 0.046\times10^{2}T^{-1} - 4.226$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf° = -19.809 + 2.037\times10^{-3}T - 3.243\times10^{-6}T^{2} + 26.900T^{-1}$
$\Delta Gf° = -19.809 - 2.037\times10^{-3}T\ln T + 3.243\times10^{-6}T^{2} + 13.450T^{-1} + 14.121\times10^{-3}T$
1043-1185 K: $\Delta Hf° = 3.752 - 41.944\times10^{-3}T + 17.468\times10^{-6}T^{2} - 201.600T^{-1}$
$\Delta Gf° = 3.752 + 41.944\times10^{-3}T\ln T - 17.468\times10^{-6}T^{2} - 100.800T^{-1} - 292.424\times10^{-3}T$
1185-1200 K: $\Delta Hf° = -19.862 - 3.689\times10^{-3}T + 1.777\times10^{-6}T^{2} - 82.600T^{-1}$
$\Delta Gf° = -19.862 + 3.689\times10^{-3}T\ln T - 1.777\times10^{-6}T^{2} - 41.300T^{-1} - 20.383\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Other data from Hultgren (210).

$Fe_3Si(c)$
Triiron Silicide
[Formation: $3Fe(c) + Si(c) = Fe_3Si(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	23.480	24.760	24.760	0	-22.400	-22.609	16.572
300	23.500	24.910	24.767	.043	-22.399	-22.612	16.472
400	25.320	31.920	25.710	2.484	-22.343	-22.694	12.399
500	27.280	37.800	27.560	5.120	-22.299	-22.790	9.961
600	29.360	42.920	29.680	7.944	-22.258	-22.877	8.333
700	31.400	47.640	31.931	10.996	-22.182	-22.999	7.180
800	36.640	52.000	34.150	14.280	-22.098	-23.104	6.312
830	60.000	53.640	34.801	15.636	-21.759	-23.129	6.090
900	33.480	56.640	36.418	18.200	-21.684	-23.279	5.653
1000	35.200	60.240	38.608	21.632	-22.288	-23.408	5.116
1043	36.507	61.749	39.531	23.174	-22.921	-23.445	4.913
1100	38.240	63.720	40.735	25.284	-23.269	-23.468	4.663
1185	40.994	66.641	42.468	28.645	-23.107	-23.463	4.327
1185	40.994	66.641	42.468	28.645	-23.752	-23.463	4.327
1200	41.480	67.160	42.773	29.264	-23.596	-23.464	4.273
1300	44.320	70.600	44.791	33.552	-22.418	-23.509	3.952

Phase changes: 830 K, Curie temperature of Fe_3Si; $\Delta H^\circ = 0$ kcal/mol.
1043 K, Curie temperature of Fe; $\Delta H^\circ = 0$ kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H^\circ = 0.215$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-830 K: $Cp^\circ = 10.412 + 31.278\text{x}10^{-3}T + 3.327\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.412\text{x}10^{-3}T + 15.639\text{x}10^{-6}T^{2} - 3.327\text{x}10^{2}T^{-1} - 3.379$
830-1300 K: $Cp^\circ = 36.373 + 0.452\text{x}10^{-3}T$
$H^\circ - H^\circ_{298} = 36.373\text{x}10^{-3}T + 0.226\text{x}10^{-6}T^{2} - 14.709$

Formation equations (kcal/mol):

298.15-830 K: $\Delta Hf^\circ = -24.602 + 5.396\text{x}10^{-3}T - 2.925\text{x}10^{-6}T^{2} + 254.300T^{-1}$
$\Delta Gf^\circ = -24.602 - 5.396\text{x}10^{-3}T\ln T + 2.925\text{x}10^{-6}T^{2} + 127.150T^{-1} + 35.126\text{x}10^{-3}T$
830-1043 K: $\Delta Hf^\circ = -35.932 + 31.357\text{x}10^{-3}T - 18.338\text{x}10^{-6}T^{2} + 587.000T^{-1}$
$\Delta Gf^\circ = -35.932 - 31.357\text{x}10^{-3}T\ln T + 18.338\text{x}10^{-6}T^{2} + 293.500T^{-1} + 210.238\text{x}10^{-3}T$
1043-1185 K: $\Delta Hf^\circ = 34.750 - 100.586\text{x}10^{-3}T + 43.795\text{x}10^{-6}T^{2} - 98.500T^{-1}$
$\Delta Gf^\circ = 34.750 + 100.586\text{x}10^{-3}T\ln T - 43.795\text{x}10^{-6}T^{2} - 49.250T^{-1} - 709.395\text{x}10^{-3}T$
1185-1300 K: $\Delta Hf^\circ = -36.091 + 14.179\text{x}10^{-3}T - 3.278\text{x}10^{-6}T^{2} + 258.500T^{-1}$
$\Delta Gf^\circ = -36.091 - 14.179\text{x}10^{-3}T\ln T + 3.278\text{x}10^{-6}T^{2} + 129.250T^{-1} + 106.727\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Other data from Hultgren (210).

Fe_2SiO_4(c,l)
Iron Silicate, Fayalite
[Formation: 2Fe(c,l) + Si(c,l) + $2O_2$(g) = Fe_2SiO_4(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	31.525	36.090	36.090	0	-353.700	-330.009	241.900
300	31.641	36.285	36.092	.058	-353.699	-329.862	240.301
400	36.150	46.100	37.400	3.480	-353.456	-321.949	175.902
500	38.631	54.453	39.997	7.228	-353.080	-314.113	137.297
600	40.369	61.658	43.020	11.183	-352.681	-306.356	111.589
700	41.756	67.988	46.144	15.291	-352.310	-298.665	93.246
800	42.956	73.643	49.233	19.528	-352.004	-291.024	79.503
900	44.047	78.767	52.236	23.878	-351.826	-283.414	68.822
1000	45.070	83.461	55.126	28.335	-351.923	-275.804	60.276
1043	45.491	85.367	56.334	30.282	-352.236	-272.526	57.104
1100	46.049	87.803	57.902	32.891	-352.346	-268.171	53.280
1185	46.856	91.260	60.172	36.839	-352.153	-261.673	48.260
1185	46.856	91.260	60.172	36.839	-352.583	-261.673	48.260
1200	46.999	91.850	60.564	37.543	-352.476	-260.525	47.447
1300	47.927	95.649	63.118	42.290	-351.731	-252.891	42.514
1400	48.840	99.234	65.571	47.128	-350.960	-245.313	38.295
1490	49.651	102.302	67.698	51.560	-350.238	-238.556	34.990
1490	57.300	117.188	67.698	73.740	-328.058	-238.556	34.990
1500	57.300	117.571	68.029	74.313	-327.900	-237.956	34.670
1600	57.300	121.269	71.242	80.043	-326.354	-232.010	31.691
1667	57.300	123.620	73.301	83.882	-325.350	-228.059	29.899
1667	57.300	123.620	73.301	83.882	-325.750	-228.059	29.899
1687	57.300	124.303	73.901	85.028	-325.486	-226.891	29.393
1687	57.300	124.303	73.901	85.028	-337.568	-226.891	29.393
1700	57.300	124.743	74.288	85.773	-337.389	-226.034	29.058

Phase changes:
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1490 K, incongruent melting point of Fe_2SiO_4; ΔH° = 22.180 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1490 K: $Cp° = 37.474 + 8.362\times10^{-3}T - 7.505\times10^{5}T^{-2}$
$H° - H°_{298} = 37.474\times10^{-3}T + 4.181\times10^{-6}T^{2} + 7.505\times10^{2}T^{-1} - 14.062$
1490-1700 K: $Cp° = 57.300$
$H° - H°_{298} = 57.300\times10^{-3}T - 11.637$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf° = -361.588 + 17.777\times10^{-3}T - 9.318\times10^{-6}T^{2} + 1018.600T^{-1}$
$\Delta Gf° = -361.588 - 17.777\times10^{-3}T\ln T + 9.318\times10^{-6}T^{2} + 509.300T^{-1} + 198.696\times10^{-3}T$
1043-1185 K: $\Delta Hf° = -314.467 - 70.185\times10^{-3}T + 32.104\times10^{-6}T^{2} + 561.600T^{-1}$
$\Delta Gf° = -314.467 + 70.185\times10^{-3}T\ln T - 32.104\times10^{-6}T^{2} + 280.800T^{-1} - 414.393\times10^{-3}T$
1185-1490 K: $\Delta Hf° = -361.694 + 6.325\times10^{-3}T + 0.722\times10^{-6}T^{2} + 799.600T^{-1}$
$\Delta Gf° = -361.694 - 6.325\times10^{-3}T\ln T - 0.722\times10^{-6}T^{2} + 399.800T^{-1} + 129.689\times10^{-3}T$
1490-1667 K: $\Delta Hf° = -359.269 + 26.151\times10^{-3}T - 3.459\times10^{-6}T^{2} + 49.100T^{-1}$
$\Delta Gf° = -359.269 - 26.151\times10^{-3}T\ln T + 3.459\times10^{-6}T^{2} + 24.550T^{-1} + 266.860\times10^{-3}T$
1667-1687 K: $\Delta Hf° = -525.059 + 123.145\times10^{-3}T - 22.721\times10^{-6}T^{2} + 95447.500T^{-1}$
$\Delta Gf° = -525.059 - 123.145\times10^{-3}T\ln T + 22.721\times10^{-6}T^{2} + 47723.750T^{-1} + 1036.616\times10^{-3}T$
1687-1700 K: $\Delta Hf° = -537.488 + 122.724\times10^{-3}T - 22.370\times10^{-6}T^{2} + 95546.000T^{-1}$
$\Delta Gf° = -537.488 - 122.724\times10^{-3}T\ln T + 22.370\times10^{-6}T^{2} + 47773.000T^{-1} + 1041.431\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Low-temperature heat capacities and entropy at 298 K from Robie (425). High-temperature data based on Orr (375).

$FeTe_{0.90}(c)$

Iron Telluride

[Reaction: $Fe(c) + 0.45Te_2(g) = FeTe_{0.90}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	11.870	19.140	19.140	0	-22.799	-18.260	13.385
300*	11.890	19.210	19.140	.022	-22.795	-18.231	13.281
400	12.450	22.720	19.615	1.242	-22.596	-16.742	9.147
500	12.760	25.530	20.524	2.503	-22.420	-15.298	6.687
600	12.980	27.880	21.562	3.791	-22.280	-13.886	5.058
700	13.150	29.890	22.609	5.097	-22.187	-12.493	3.901
800	13.290	31.660	23.636	6.419	-22.156	-11.117	3.037
900	13.430	33.230	24.612	7.756	-22.214	-9.731	2.363
1000	13.550	34.650	25.545	9.105	-22.441	-8.334	1.821
1043	13.602	35.222	25.932	9.689	-22.682	-7.723	1.618
1100	13.670	35.950	26.435	10.466	-22.858	-6.901	1.371
1185	13.764	36.967	27.151	11.631	-22.963	-5.659	1.044
1185	13.764	36.967	27.151	11.631	-23.178	-5.659	1.044
1200	13.780	37.140	27.275	11.838	-23.162	-5.438	.990

*Data above 298 K estimated.

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 12.633 + 1.012\times10^{-3}T - 0.946\times10^{5}T^{-2}$
$H°- H°_{298} = 12.633\times10^{-3}T + 0.506\times10^{-6}T^{2} + 0.946\times10^{2}T^{-1} - 4.129$

Reaction equations (kcal/mol):

298.15-1043 K: $\Delta Hr° = -26.006 + 8.984\times10^{-3}T - 5.832\times10^{-6}T^{2} + 312.210T^{-1}$
$\Delta Gr° = -26.006 - 8.984\times10^{-3}T\ln T + 5.832\times10^{-6}T^{2} + 156.105T^{-1} + 73.674\times10^{-3}T$

1043-1185 K: $\Delta Hr° = -2.445 - 34.997\times10^{-3}T + 14.879\times10^{-6}T^{2} + 83.710T^{-1}$
$\Delta Gr° = -2.445 + 34.997\times10^{-3}T\ln T - 14.879\times10^{-6}T^{2} + 41.855T^{-1} - 232.870\times10^{-3}T$

1185-1200 K: $\Delta Hr° = -26.059 + 3.258\times10^{-3}T - 0.812\times10^{-6}T^{2} + 202.710T^{-1}$
$\Delta Gr° = -26.059 - 3.258\times10^{-3}T\ln T + 0.812\times10^{-6}T^{2} + 101.355T^{-1} + 39.171\times10^{-3}T$

Source: Data from Mills (332) who estimated all above 298 K.

$FeTe_2(c)$
Iron Ditelluride
[Reaction: $Fe(c) + Te_2(g) = FeTe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	17.620	23.940	23.940	0	-55.630	-42.377	31.063
300*	17.640	24.050	23.943	.032	-55.625	-42.297	30.813
400	18.620	29.270	24.648	1.849	-55.313	-37.899	20.707
500	19.340	33.500	26.004	3.748	-54.992	-33.581	14.678
600	19.950	37.090	27.567	5.714	-54.676	-29.328	10.683
700	20.520	40.200	29.147	7.737	-54.377	-25.123	7.844
800	21.060	42.980	30.710	9.816	-54.109	-20.970	5.729
900	21.580	45.490	32.214	11.948	-53.900	-16.842	4.090
933	21.750	46.270	32.698	12.663	-53.860	-15.483	3.627

*Data above 298 K estimated.

Phase change: 933 K, melting point of $FeTe_2$; ΔH° unknown

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-933 K: $Cp° = 17.284 + 4.912\times10^{-3}T - 1.002\times10^{5}T^{-2}$

$H°-H°_{298} = 17.284\times10^{-3}T + 2.456\times10^{-6}T^{2} + 1.002\times10^{2}T^{-1} - 5.708$

Reaction equations (kcal/mol):

298.15-933 K: $\Delta Hr° = -58.933 + 8.906\times10^{-3}T - 4.208\times10^{-6}T^{2} + 304.500T^{-1}$

$\Delta Gr° = -58.933 - 8.906\times10^{-3}T\ln T + 4.208\times10^{-6}T^{2} + 152.250T^{-1} + 103.302\times10^{-3}T$

Source: Data from Mills (332) who estimated all above 298 K.

$FeTiO_3$(c,l)
Iron Titanium Trioxide, Ilmenite
[Formation: $Fe(c,l) + Ti(c,l) + 1.5O_2(g) = FeTiO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	23.780	25.300	25.300	0	-295.600	-277.101	203.118
300	23.858	25.447	25.300	.044	-295.598	-276.984	201.780
400	26.669	32.773	26.280	2.597	-295.352	-270.813	147.964
500	28.014	38.880	28.208	5.336	-295.034	-264.717	115.706
600	28.994	44.077	30.430	8.188	-294.716	-258.683	94.224
700	29.853	48.612	32.711	11.131	-294.423	-252.694	78.894
800	30.637	52.651	34.956	14.156	-294.173	-246.755	67.409
900	31.338	56.301	37.128	17.256	-293.995	-240.837	58.483
1000	31.938	59.634	39.213	20.421	-293.964	-234.933	51.344
1043	32.150	60.983	40.083	21.799	-294.093	-232.393	48.695
1100	32.432	62.702	41.211	23.640	-294.119	-229.025	45.502
1156	32.658	64.319	42.292	25.463	-294.045	-225.710	42.671
1156	32.658	64.319	42.292	25.463	-295.062	-225.710	42.671
1185	32.775	65.129	42.841	26.412	-294.980	-223.970	41.306
1185	32.775	65.129	42.841	26.412	-295.195	-223.970	41.306
1200	32.835	65.542	43.122	26.904	-295.123	-223.071	40.626
1300	33.186	68.184	44.949	30.205	-294.647	-217.085	36.495
1400	33.551	70.657	46.698	33.542	-294.188	-211.137	32.960
1500	34.024	72.987	48.374	36.919	-293.737	-205.221	29.900
1600	34.727	75.203	49.982	40.354	-293.280	-199.334	27.227
1640	35.105	76.066	50.608	41.750	-293.090	-196.990	26.251
1640	47.600	89.279	50.608	63.420	-271.420	-196.990	26.251
1667	47.600	90.056	51.241	64.705	-270.953	-195.767	25.665
1667	47.600	90.056	51.241	64.705	-271.153	-195.767	25.665
1700	47.600	90.989	52.003	66.276	-270.614	-194.279	24.976
1800	47.600	93.710	54.246	71.036	-269.022	-189.835	23.049
1811	47.600	94.000	54.486	71.560	-268.854	-189.354	22.851
1811	47.600	94.000	54.486	71.560	-272.154	-189.354	22.851
1900	47.600	96.283	56.390	75.796	-270.869	-185.315	21.316
1945	47.600	97.397	57.326	77.938	-270.235	-183.297	20.596
1945	47.600	97.397	57.326	77.938	-273.535	-183.297	20.596
2000	47.600	98.725	58.447	80.556	-272.872	-180.756	19.752

Phase changes:
1043 K, Curie temperature of Fe; $\Delta H^\circ = 0$ kcal/mol.
1156 K, α - β transition point of Ti; $\Delta H^\circ = 1.017$ kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H^\circ = 0.215$ kcal/mol.
1640 K, melting point of $FeTiO_3$; $\Delta H^\circ = 21.670$ kcal/mol.
1667 K, γ - δ transition point of Fe; $\Delta H^\circ = 0.200$ kcal/mol.
1811 K, melting point of Fe; $\Delta H^\circ = 3.300$ kcal/mol.
1945 K, melting point of Ti; $\Delta H^\circ = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1640 K: $C_p^\circ = 27.890 + 4.340\times10^{-3}T - 4.802\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 27.890\times10^{-3}T + 2.170\times10^{-6}T^2 + 4.802\times10^{2}T^{-1} - 10.119$
1640-2000 K: $C_p^\circ = 47.600$
$H^\circ - H^\circ_{298} = 47.600\times10^{-3}T - 14.644$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -300.701 + 11.789\times10^{-3}T - 5.779\times10^{-6}T^2 + 626.100T^{-1}$
$\Delta Gf^\circ = -300.701 - 11.789\times10^{-3}T\ln T + 5.779\times10^{-6}T^2 + 313.050T^{-1} + 141.081\times10^{-3}T$
1043-1156 K: $\Delta Hf^\circ = -277.140 - 32.192\times10^{-3}T + 14.932\times10^{-6}T^2 + 397.600T^{-1}$
$\Delta Gf^\circ = -277.140 + 32.192\times10^{-3}T\ln T - 14.932\times10^{-6}T^2 + 198.800T^{-1} - 165.463\times10^{-3}T$
1156-1185 K: $\Delta Hf^\circ = -281.177 - 29.792\times10^{-3}T + 14.609\times10^{-6}T^2 + 1180.500T^{-1}$
$\Delta Gf^\circ = -281.177 + 29.792\times10^{-3}T\ln T - 14.609\times10^{-6}T^2 + 590.250T^{-1} - 145.711\times10^{-3}T$
1185-1640 K: $\Delta Hf^\circ = -304.791 + 8.463\times10^{-3}T - 1.081\times10^{-6}T^2 + 1299.500T^{-1}$
$\Delta Gf^\circ = -304.791 - 8.463\times10^{-3}T\ln T + 1.081\times10^{-6}T^2 + 649.750T^{-1} + 126.330\times10^{-3}T$
1640-1667 K: $\Delta Hf^\circ = -309.316 + 28.173\times10^{-3}T - 3.251\times10^{-6}T^2 + 819.300T^{-1}$
$\Delta Gf^\circ = -309.316 - 28.173\times10^{-3}T\ln T + 3.251\times10^{-6}T^2 + 409.650T^{-1} + 271.522\times10^{-3}T$
1667-1811 K: $\Delta Hf^\circ = -392.211 + 76.670\times10^{-3}T - 12.883\times10^{-6}T^2 + 48518.500T^{-1}$
$\Delta Gf^\circ = -392.211 - 76.670\times10^{-3}T\ln T + 12.883\times10^{-6}T^2 + 24259.250T^{-1} + 656.400\times10^{-3}T$
1811-1945 K: $\Delta Hf^\circ = -306.361 + 22.678\times10^{-3}T - 2.201\times10^{-6}T^2 + 700.300T^{-1}$
$\Delta Gf^\circ = -306.361 - 22.678\times10^{-3}T\ln T + 2.201\times10^{-6}T^2 + 350.150T^{-1} + 230.603\times10^{-3}T$
1945-2000 K: $\Delta Hf^\circ = -299.229 + 14.705\times10^{-3}T - 0.754\times10^{-6}T^2 - 67.800T^{-1}$
$\Delta Gf^\circ = -299.229 - 14.705\times10^{-3}T\ln T + 0.754\times10^{-6}T^2 - 33.900T^{-1} + 169.470\times10^{-3}T$

Sources: Enthalpy of formaiton based on Kelley (249), Levitskii (304), and Levitskii (306). Low-temperature heat capacities and entropy at 298 K from Shomate (452). High-temperature data based on Naylor (353).

$Fe_2TiO_4(c)$
Diiron Titanium Tetroxide
[Formation: $2Fe(c) + Ti(c) + 2O_2(g) = Fe_2TiO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	34.010	40.400	40.400	0	-362.000	-338.753	248.310
300	34.186	40.611	40.401	.063	-361.996	-338.608	246.672
400	37.684	50.974	41.789	3.674	-361.673	-330.855	180.769
500	39.911	59.637	44.517	7.560	-361.256	-323.201	141.269
600	41.615	67.069	47.671	11.639	-360.825	-315.629	114.966
700	43.079	73.596	50.917	15.875	-360.424	-308.121	96.199
800	44.448	79.438	54.123	20.252	-360.086	-300.678	82.140
900	45.818	84.752	57.235	24.765	-359.863	-293.265	71.214
1000	47.263	89.654	60.236	29.418	-359.894	-285.868	62.476
1043	47.944	91.658	61.490	31.465	-360.167	-282.681	59.232
1100	48.846	94.231	63.120	34.222	-360.215	-278.447	55.322
1156	49.841	96.680	64.688	36.983	-360.031	-274.286	51.855
1156	49.841	96.680	64.688	36.983	-361.048	-274.286	51.855
1185	50.356	97.921	65.486	38.436	-360.879	-272.111	50.185
1185	50.356	97.921	65.486	38.436	-361.309	-272.111	50.185
1200	50.623	98.556	65.895	39.193	-361.157	-270.985	49.353
1300	52.648	102.686	68.567	44.355	-360.068	-263.512	44.300
1400	54.975	106.671	71.147	49.733	-358.841	-256.131	39.983
1500	57.653	110.553	73.646	55.361	-357.435	-248.843	36.256
1600	60.734	114.370	76.072	61.277	-355.817	-241.654	33.008

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 33.789 + 14.564\times10^{-3}T - 3.663\times10^{5}T^{-2}$
$H°-H°_{298} = 33.789\times10^{-3}T + 7.282\times10^{-6}T^{2} + 3.663\times10^{2}T^{-1} - 11.950$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf° = -368.049 + 14.294\times10^{-3}T - 6.989\times10^{-6}T^{2} + 718.100T^{-1}$
$\Delta Gf° = -368.049 - 14.294\times10^{-3}T\ln T + 6.989\times10^{-6}T^{2} + 359.050T^{-1} + 173.577\times10^{-3}T$
1043-1156 K: $\Delta Hf° = -320.927 - 73.668\times10^{-3}T + 34.433\times10^{-6}T^{2} + 261.100T^{-1}$
$\Delta Gf° = -320.927 + 73.668\times10^{-3}T\ln T - 34.433\times10^{-6}T^{2} + 130.550T^{-1} - 439.512\times10^{-3}T$
1156-1185 K: $\Delta Hf° = -324.964 - 71.268\times10^{-3}T + 34.110\times10^{-6}T^{2} + 1044.000T^{-1}$
$\Delta Gf° = -324.964 + 71.268\times10^{-3}T\ln T - 34.110\times10^{-6}T^{2} + 522.000T^{-1} - 419.759\times10^{-3}T$
1185-1600 K: $\Delta Hf° = -372.192 + 5.242\times10^{-3}T + 2.728\times10^{-6}T^{2} + 1282.000T^{-1}$
$\Delta Gf° = -372.192 - 5.242\times10^{-3}T\ln T - 2.728\times10^{-6}T^{2} + 641.000T^{-1} + 124.322\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Levitskii (305). Low-temperature heat capacities from Todd (496). Entropy at 298 K from Kelley (246). High-temperature data based on Bonnickson (52).

$Fe_2TiO_5(c)$

Diiron Titanium Pentoxide

[Formation: $2Fe(c) + Ti(c) + 2.5O_2(g) = Fe_2TiO_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	39.260	37.400	37.400	0	-419.100	-387.653	284.154
300	39.372	37.643	37.400	.073	-419.092	-387.456	282.258
400	43.503	49.608	39.003	4.242	-418.566	-376.984	205.972
500	45.711	59.573	42.149	8.712	-417.931	-366.663	160.266
600	47.157	68.043	45.778	13.359	-417.310	-356.469	129.842
700	48.245	75.397	49.496	18.131	-416.762	-346.366	108.139
800*	49.140	81.899	53.147	23.002	-416.328	-336.345	91.884
900	49.924	87.733	56.671	27.956	-416.072	-326.363	79.251
1000	50.639	93.031	60.047	32.984	-416.141	-316.397	69.148
1043	50.927	95.169	61.451	35.168	-416.457	-312.103	65.397
1100	51.309	97.889	63.269	38.082	-416.587	-306.398	60.875
1156	51.667	100.446	65.008	40.965	-416.518	-300.787	56.865
1156	51.667	100.446	65.008	40.965	-417.535	-300.787	56.865
1185	51.852	101.728	65.891	42.466	-417.440	-297.860	54.934
1185	51.852	101.728	65.891	42.466	-417.870	-297.860	54.934
1200	51.948	102.381	66.343	43.245	-417.762	-296.343	53.971
1300	52.565	106.563	69.278	48.471	-417.036	-286.252	48.123
1400	53.166	110.481	72.083	53.757	-416.334	-276.221	43.119
1500	53.756	114.169	74.766	59.104	-415.643	-266.235	38.790
1600	54.337	117.657	77.340	64.508	-414.976	-256.297	35.008
1667	54.722	119.894	79.005	68.162	-414.538	-249.661	32.731
1667	54.722	119.894	79.005	68.162	-414.938	-249.661	32.731
1700	54.912	120.969	79.810	69.971	-414.778	-246.391	31.675
1800	55.480	124.123	82.184	75.491	-414.314	-236.496	28.714

*Some evidence indicates Fe_2TiO_5 is metastable with respect to the oxides below 850 K, Navrotsky (348).

Phase changes:
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 45.968 + 5.412\times10^{-3}T - 7.407\times10^{5}T^{-2}$
$H°-H°_{298} = 45.968\times10^{-3}T + 2.706\times10^{-6}T^{2} + 7.407\times10^{2}T^{-1} - 16.430$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf° = -428.453 + 22.858\times10^{-3}T - 11.817\times10^{-6}T^{2} + 1069.900T^{-1}$
$\Delta Gf° = -428.453 - 22.858\times10^{-3}T\ln T + 11.817\times10^{-6}T^{2} + 534.950T^{-1} + 257.538\times10^{-3}T$
1043-1156 K: $\Delta Hf° = -381.332 - 65.104\times10^{-3}T + 29.605\times10^{-6}T^{2} + 612.900T^{-1}$
$\Delta Gf° = -381.332 + 65.104\times10^{-3}T\ln T - 29.605\times10^{-6}T^{2} + 306.450T^{-1} - 355.551\times10^{-3}T$
1156-1185 K: $\Delta Hf° = -385.369 - 62.704\times10^{-3}T + 29.282\times10^{-6}T^{2} + 1395.800T^{-1}$
$\Delta Gf° = -385.369 + 62.704\times10^{-3}T\ln T - 29.282\times10^{-6}T^{2} + 697.900T^{-1} - 335.799\times10^{-3}T$
1185-1667 K: $\Delta Hf° = -432.596 + 13.806\times10^{-3}T - 2.099\times10^{-6}T^{2} + 1633.800T^{-1}$
$\Delta Gf° = -432.596 - 13.806\times10^{-3}T\ln T + 2.099\times10^{-6}T^{2} + 816.900T^{-1} + 208.283\times10^{-3}T$
1667-1800 K: $\Delta Hf° = -598.386 + 110.800\times10^{-3}T - 21.361\times10^{-6}T^{2} + 97032.200T^{-1}$
$\Delta Gf° = -598.386 - 110.800\times10^{-3}T\ln T + 21.361\times10^{-6}T^{2} + 48516.100T^{-1} + 978.040\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Navrotsky (348). Low-temperature heat capacities and entropy at 298 K from Todd (496). High-temperature data based on Bonnickson (52).

$FeWO_4(c)$
Iron Tungstate
[Formation: $Fe(c) + W(c) + 2O_2(g) = FeWO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	27.660	31.610	31.610	0	-280.000	-255.933	187.602
300	27.740	31.780	31.613	.050	-279.998	-255.784	186.336
400	31.250	40.290	32.740	3.020	-279.665	-247.751	135.363
500	33.460	47.520	35.000	6.260	-279.175	-239.832	104.829
600*	34.790	53.740	37.607	9.680	-278.620	-232.012	84.509
700	35.620	59.170	40.313	13.200	-278.077	-224.287	70.025
800	36.230	63.970	42.983	16.790	-277.580	-216.649	59.185
900	36.760	68.270	45.559	20.440	-277.161	-209.054	50.765
1000	37.230	72.170	48.030	24.140	-276.896	-201.506	44.039
1043	37.432	73.742	49.058	25.745	-276.924	-198.264	41.544
1100	37.700	75.750	50.395	27.890	-276.809	-193.965	38.537
1185	38.091	78.570	52.310	31.118	-276.468	-187.575	34.594
1185	38.091	78.570	52.310	31.118	-276.683	-187.575	34.594
1200	38.160	79.050	52.642	31.690	-276.588	-186.449	33.957
1300	38.560	82.120	54.797	35.520	-275.959	-178.962	30.086

*Data extrapolated above 530 K.

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 34.371 + 3.588\text{x}10^{-3}T - 6.917\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 34.371\text{x}10^{-3}T + 1.794\text{x}10^{-6}T^{2} + 6.917\text{x}10^{2}T^{-1} - 12.727$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -286.479 + 14.317\text{x}10^{-3}T - 5.654\text{x}10^{-6}T^{2} + 808.800T^{-1}$
$\Delta Gf^\circ = -286.479 - 14.317\text{x}10^{-3}T\ln T + 5.654\text{x}10^{-6}T^{2} + 404.400T^{-1} + 177.787\text{x}10^{-3}T$
1043-1185 K: $\Delta Hf^\circ = -262.918 - 29.664\text{x}10^{-3}T + 15.057\text{x}10^{-6}T^{2} + 580.300T^{-1}$
$\Delta Gf^\circ = -262.918 + 29.664\text{x}10^{-3}T\ln T - 15.057\text{x}10^{-6}T^{2} + 290.150T^{-1} - 128.757\text{x}10^{-3}T$
1185-1300 K: $\Delta Hf^\circ = -286.532 + 8.591\text{x}10^{-3}T - 0.634\text{x}10^{-6}T^{2} + 699.300T^{-1}$
$\Delta Gf^\circ = -286.532 - 8.591\text{x}10^{-3}T\ln T + 0.634\text{x}10^{-6}T^{2} + 349.650T^{-1} + 143.284\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Rezukhina (424) and Kleykamp (275). Low-temperature heat capacities to 530 K and entropy at 298 K from Lyon (314). Data extrapolated above 530 K.

$GaAs(c,l)$
Gallium Arsenide
[Formation: $Ga(c,l) + As[a,1/4As_4(g)] = GaAs(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.182	15.340	15.340	0	-21.000	-20.120	14.748
300	11.194	15.410	15.343	.020	-21.003	-20.116	14.654
302.9	11.208	15.518	15.344	.052	-21.007	-20.108	14.508
302.9	11.208	15.518	15.344	.052	-22.343	-20.108	14.508
400	11.660	18.700	15.785	1.166	-22.452	-19.372	10.584
500	11.860	21.324	16.640	2.342	-22.533	-18.591	8.126
600	12.150	23.512	17.609	3.542	-22.599	-17.797	6.483
700	12.434	25.406	18.589	4.772	-22.645	-16.992	5.305
800	12.714	27.086	19.549	6.030	-22.675	-16.182	4.421
876	12.924	28.248	20.253	7.003	-22.690	-15.566	3.884
876	12.924	28.248	20.253	7.003	-30.999	-15.566	3.884
900	12.990	28.598	20.471	7.314	-30.958	-15.144	3.677
1000	13.264	29.982	21.354	8.628	-30.772	-13.397	2.928
1100	13.532	31.258	22.198	9.966	-30.563	-11.671	2.319
1200	13.798	32.448	23.003	11.334	-30.324	-9.964	1.815
1300	14.060	33.562	23.773	12.726	-30.062	-8.277	1.391
1400	14.320	34.614	24.510	14.146	-29.772	-6.612	1.032
1500	14.576	35.610	25.217	15.590	-29.458	-4.968	.724
1513*	14.608	35.736	25.306	15.780	-29.415	-4.755	.687
1513	15.000	52.378	25.306	40.960	-4.235	-4.755	.687
1600	15.000	53.218	26.802	42.266	-3.912	-4.795	.655

*Heat capacity of liquid estimated.

Phase changes: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.
876 K, sublimation point of As to $As_4(g)$; ΔH° = 33.235 kcal/mol of $As_4(g)$.
1513 K, melting point of GaAs; ΔH° = 25.180 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1513 K: $Cp^\circ = 10.725 + 2.568\times10^{-3}T - 0.275\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.725\times10^{-3}T + 1.284\times10^{-6}T^2 + 0.275\times10^{2}T^{-1} - 3.404$
1513-1600 K: $Cp^\circ = 15.000$
$H^\circ - H^\circ_{298} = 15.000\times10^{-3}T + 18.265$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf^\circ = -20.669 - 1.462\times10^{-3}T + 0.613\times10^{-6}T^2 + 15.100T^{-1}$
$\Delta Gf^\circ = -20.669 + 1.462\times10^{-3}T\ln T - 0.613\times10^{-6}T^2 + 7.550T^{-1} - 6.389\times10^{-3}T$
302.9-876 K: $\Delta Hf^\circ = -22.375 - 0.966\times10^{-3}T + 0.587\times10^{-6}T^2 + 82.300T^{-1}$
$\Delta Gf^\circ = -22.375 + 0.966\times10^{-3}T\ln T - 0.587\times10^{-6}T^2 + 41.150T^{-1} + 1.702\times10^{-3}T$
876-1513 K: $\Delta Hf^\circ = -31.703 - 0.268\times10^{-3}T + 1.165\times10^{-6}T^2 + 50.800T^{-1}$
$\Delta Gf^\circ = -31.703 + 0.268\times10^{-3}T\ln T - 1.165\times10^{-6}T^2 + 25.400T^{-1} + 17.606\times10^{-3}T$
1513-1600 K: $\Delta Hf^\circ = -10.034 + 4.007\times10^{-3}T - 0.119\times10^{-6}T^2 + 23.300T^{-1}$
$\Delta Gf^\circ = -10.034 - 4.007\times10^{-3}T\ln T + 0.119\times10^{-6}T^2 + 11.650T^{-1} + 32.648\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Brebrick (55), Foxon (155), Panish (380), and Pupp (411). Low-temperature heat capacities and entropy at 298 K from Piesbergen (400). High-temperature data based on Dash (108) and Lichter (309). Heat capacity of liquid estimated.

GaH(g)
Gallium Hydride (ideal gas)
[Formation: $Ga(c,l) + 0.5H_2(g) = GaH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.036	47.721	47.721	0	51.219	44.553	-32.657
300	7.038	47.765	47.722	.013	51.214	44.511	-32.426
302.9	7.043	47.833	47.722	.033	51.205	44.445	-32.068
302.9	7.043	47.833	47.722	.033	49.869	44.445	-32.068
400	7.221	49.812	48.000	.725	49.583	42.750	-23.357
500	7.469	51.450	48.532	1.459	49.324	41.073	-17.953
600	7.721	52.834	49.136	2.219	49.095	39.445	-14.368
700	7.949	54.042	49.752	3.003	48.892	37.853	-11.818
800	8.143	55.116	50.356	3.808	48.709	36.289	-9.914
900	8.307	56.085	50.941	4.630	48.541	34.746	-8.437
1000	8.445	56.968	51.500	5.468	48.385	33.222	-7.260
1100	8.561	57.778	52.033	6.319	48.238	31.713	-6.301
1200	8.662	58.527	52.544	7.180	48.096	30.217	-5.503
1300	8.749	59.224	53.032	8.050	47.958	28.733	-4.830
1400	8.826	59.876	53.498	8.929	47.824	27.258	-4.255
1500	8.896	60.487	53.944	9.815	47.691	25.793	-3.758
1600	8.960	61.063	54.370	10.708	47.561	24.338	-3.324
1700	9.019	61.608	54.780	11.607	47.431	22.892	-2.943
1800	9.076	62.125	55.174	12.512	47.303	21.452	-2.605
1900	9.130	62.617	55.553	13.422	47.174	20.019	-2.303
2000	8.944	63.087	55.918	14.338	47.048	18.593	-2.032

Phase change: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.160 + 1.192\times10^{-3}T - 0.426\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.160\times10^{-3}T + 0.596\times10^{-6}T^2 + 0.426\times10^{2}T^{-1} - 2.331$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf^\circ = 51.787 - 2.564\times10^{-3}T + 0.287\times10^{-6}T^2 + 50.850T^{-1}$

$\Delta Gf^\circ = 51.787 + 2.564\times10^{-3}T\ln T - 0.287\times10^{-6}T^2 + 25.425T^{-1} - 39.075\times10^{-3}T$

302.9-2000 K: $\Delta Hf^\circ = 50.082 - 2.068\times10^{-3}T + 0.261\times10^{-6}T^2 + 118.050T^{-1}$

$\Delta Gf^\circ = 50.082 + 2.068\times10^{-3}T\ln T - 0.261\times10^{-6}T^2 + 59.025T^{-1} - 30.984\times10^{-3}T$

Source: Data from Gurvich (196).

GaN(c)
Gallium Nitride
[Formation: $Ga(c,l) + 0.5N_2(g) = GaN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.341	8.724	8.724	0	-26.400	-19.269	14.124
300*	8.381	8.776	8.726	.015	-26.403	-19.225	14.005
302.9	8.430	8.857	8.727	.039	-26.408	-19.156	13.822
302.9	8.430	8.857	8.727	.039	-27.744	-19.156	13.822
400	10.071	11.465	9.080	.954	-27.808	-16.388	8.954
500	10.965	13.816	9.798	2.009	-27.748	-13.538	5.917
600	11.600	15.874	10.642	3.139	-27.614	-10.707	3.900
700	12.111	17.701	11.522	4.325	-27.428	-7.903	2.467
800	12.554	19.348	12.399	5.559	-27.200	-5.129	1.401
900	12.957	20.850	13.256	6.835	-26.939	-2.385	.579
1000	13.333	22.235	14.086	8.149	-26.647	.327	-.071
1100	13.692	23.523	14.886	9.501	-26.324	3.009	-.598
1200	14.036	24.729	15.656	10.887	-25.973	5.660	-1.031
1300	14.371	25.866	16.398	12.308	-25.593	8.282	-1.392
1400	14.697	26.943	17.114	13.761	-25.185	10.871	-1.697
1500	15.016	27.968	17.803	15.247	-24.749	13.432	-1.957
1600	15.330	28.947	18.470	16.764	-24.285	15.962	-2.180

*Data above 298 K estimated.

Phase change: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 10.607 + 3.012\text{x}10^{-3}T - 2.813\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 10.607\text{x}10^{-3}T + 1.506\text{x}10^{-6}T^{2} + 2.813\text{x}10^{2}T^{-1} - 4.240$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = -27.710 + 0.853\text{x}10^{-3}T + 1.111\text{x}10^{-6}T^{2} + 285.250T^{-1}$

$\Delta Gf° = -27.710 - 0.853\text{x}10^{-3}T\ln T - 1.111\text{x}10^{-6}T^{2} + 142.625T^{-1} + 31.896\text{x}10^{-3}T$

302.9-1600 K: $\Delta Hf° = -29.415 + 1.349\text{x}10^{-3}T + 1.086\text{x}10^{-6}T^{2} + 352.450T^{-1}$

$\Delta Gf° = -29.415 - 1.349\text{x}10^{-3}T\ln T - 1.086\text{x}10^{-6}T^{2} + 176.225T^{-1} + 39.987\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from Koshchenko (282). Data above 298 K estimated.

$GaO(g)$
Gallium Monoxide (ideal gas)
[Formation: $Ga(c,l) + 0.5O_2(g) = GaO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	7.690	55.158	55.158	0	40.000	33.769	-24.753
300	7.700	55.205	55.158	.014	39.995	33.730	-24.572
302.9	7.711	55.279	55.159	.036	39.989	33.669	-24.293
302.9	7.711	55.279	55.159	.036	38.653	33.669	-24.293
400	8.080	57.475	55.465	.804	38.436	32.106	-17.541
500	8.330	59.306	56.056	1.625	38.247	30.546	-13.352
600	8.500	60.843	56.730	2.468	38.073	29.022	-10.571
700	8.620	62.164	57.414	3.325	37.906	27.527	-8.594
800	8.700	63.320	58.081	4.191	37.738	26.056	-7.118
900	8.770	64.350	58.722	5.065	37.569	24.605	-5.975
1000	8.820	65.276	59.332	5.944	37.400	23.174	-5.065
1100	8.860	66.118	59.911	6.828	37.229	21.760	-4.323
1200	8.890	66.891	60.461	7.716	37.058	20.361	-3.708
1300	8.920	67.603	60.983	8.606	36.885	18.977	-3.190
1400	8.940	68.265	61.480	9.499	36.712	17.605	-2.748
1500	8.960	68.882	61.953	10.393	36.536	16.246	-2.367
1600	8.980	69.461	62.405	11.290	36.359	14.899	-2.035
1700	9.000	70.006	62.836	12.189	36.182	13.564	-1.744
1800	9.010	70.521	63.249	13.090	36.004	12.239	-1.486
1900	9.030	71.009	63.645	13.992	35.824	10.922	-1.256
2000	9.040	71.473	64.025	14.896	35.644	9.616	-1.051

Phase change: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.561 + 0.298\times10^{-3}T - 0.854\times10^{5}T^{-2}$
$H° - H°_{298} = 8.561\times10^{-3}T + 0.149\times10^{-6}T^{2} + 0.854\times10^{2}T^{-1} - 2.852$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = 40.270 - 1.550\times10^{-3}T - 0.202\times10^{-6}T^{2} + 62.800T^{-1}$
$\Delta Gf° = 40.270 + 1.550\times10^{-3}T\ln T + 0.202\times10^{-6}T^{2} + 31.400T^{-1} - 31.046\times10^{-3}T$
302.9-2000 K: $\Delta Hf° = 38.564 - 1.054\times10^{-3}T - 0.228\times10^{-6}T^{2} + 130.000T^{-1}$
$\Delta Gf° = 38.564 + 1.054\times10^{-3}T\ln T + 0.228\times10^{-6}T^{2} + 65.000T^{-1} - 22.955\times10^{-3}T$

Source: Data from Pedley (396).

$Ga_2O(g)$
Digallium Oxide (ideal gas)
[Formation: $2Ga(c,l) + 0.5O_2(g) = Ga_2O(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.737	67.982	67.982	0	-22.766	-29.911	21.925
300	11.753	68.054	67.982	.022	-22.775	-29.955	21.822
302.9	11.773	68.167	67.982	.056	-22.789	-30.026	21.664
302.9	11.773	68.167	67.982	.056	-25.461	-30.026	21.664
400	12.449	71.539	68.451	1.235	-25.906	-31.420	17.167
500	12.879	74.367	69.361	2.503	-26.292	-32.751	14.315
600	13.152	76.741	70.399	3.805	-26.646	-34.010	12.388
700	13.333	78.782	71.453	5.130	-26.982	-35.209	10.993
800	13.457	80.572	72.484	6.470	-27.311	-36.363	9.934
900	13.547	82.162	73.472	7.821	-27.637	-37.474	9.100
1000	13.612	83.593	74.414	9.179	-27.962	-38.550	8.425
1100	13.662	84.893	75.309	10.542	-28.289	-39.594	7.867
1200	13.700	86.083	76.157	11.911	-28.614	-40.608	7.396
1300	13.730	87.181	76.964	13.282	-28.941	-41.593	6.992
1400	13.754	88.200	77.731	14.656	-29.269	-42.557	6.643
1500	13.774	89.149	78.460	16.033	-29.59	-43.493	6.337
1600	13.790	90.038	79.156	17.411	-29.9	-44.408	6.066
1700	13.804	90.875	79.821	18.791	-30.2	-45.303	5.824
1800	13.815	91.664	80.457	20.172	-30.591	-46.177	5.607
1900	13.825	92.412	81.068	21.554	-30.926	-47.037	5.410
2000	13.833	93.121	81.653	22.936	-31.264	-47.875	5.232

Phase change: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.422 + 0.284\times10^{-3}T - 1.573\times10^{5}T^{-2}$

$H°- H°_{298} = 13.422\times10^{-3}T + 0.142\times10^{-6}T^{2} + 1.573\times10^{2}T^{-1} - 4.542$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = -22.241 - 3.185\times10^{-3}T - 0.309\times10^{-6}T^{2} + 134.700T^{-1}$

$\Delta Gf° = -22.241 + 3.185\times10^{-3}T\ln T + 0.309\times10^{-6}T^{2} + 67.350T^{-1} - 44.722\times10^{-3}T$

302.90-2000 K: $\Delta Hf° = -25.652 - 2.193\times10^{-3}T - 0.362\times10^{-6}T^{2} + 269.100T^{-1}$

$\Delta Gf° = -25.652 + 2.193\times10^{-3}T\ln T + 0.362\times10^{-6}T^{2} + 134.550T^{-1} - 28.540\times10^{-3}T$

Source: Data from Gurvich (196).

$GaOH(g)$
Gallium Monohydroxide (ideal gas)
[Formation: $Ga(c,l) + 0.5O_2(g) + 0.5H_2(g) = GaOH(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.296	57.165	57.165	0	-30.570	-32.747	24.004
300	11.311	57.235	57.165	.021	-30.574	-32.761	23.866
302.9	11.328	57.344	57.166	.054	-30.580	-32.782	23.653
302.9	11.328	57.344	57.166	.054	-31.916	-32.782	23.653
400	11.910	60.580	57.618	1.185	-32.107	-33.030	18.046
500	12.242	63.277	58.489	2.394	-32.257	-33.242	14.530
600	12.455	65.529	59.479	3.630	-32.388	-33.426	12.175
700	12.618	67.461	60.485	4.883	-32.511	-33.589	10.487
800	12.762	69.156	61.466	6.152	-32.628	-33.736	9.216
900	12.901	70.667	62.405	7.436	-32.742	-33.867	8.224
1000	13.036	72.033	63.300	8.733	-32.853	-33.985	7.427
1100	13.168	73.282	64.152	10.043	-32.960	-34.094	6.774
1200	13.295	74.433	64.961	11.366	-33.064	-34.193	6.227
1300	13.416	75.502	65.731	12.702	-33.164	-34.281	5.763
1400	13.529	76.500	66.465	14.049	-33.262	-34.364	5.364
1500	13.633	77.437	67.166	15.407	-33.358	-34.440	5.018
1600	13.730	78.320	67.836	16.775	-33.451	-34.510	4.714
1700	13.818	79.156	68.478	18.153	-33.543	-34.573	4.445
1800	13.898	79.948	69.093	19.539	-33.635	-34.631	4.205
1900	13.972	80.701	69.684	20.932	-33.727	-34.684	3.990
2000	14.039	81.419	70.253	22.333	-33.818	-34.730	3.795

*Data except enthalpy of formation at 298 K estimated.

Phase change: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.111 + 1.030\times10^{-3}T - 0.998\times10^{5}T^{-2}$

$H°-H°_{298} = 12.111\times10^{-3}T + 0.515\times10^{-6}T^{2} + 0.998\times10^{2}T^{-1} - 3.991$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = -30.486 - 1.228\times10^{-3}T - 0.046\times10^{-6}T^{2} + 85.450T^{-1}$

$\Delta Gf° = -30.486 + 1.228\times10^{-3}T\ln T + 0.046\times10^{-6}T^{2} + 42.725T^{-1} - 15.072\times10^{-3}T$

302.9-2000 K: $\Delta Hf° = -32.192 - 0.732\times10^{-3}T - 0.072\times10^{-6}T^{2} + 152.650T^{-1}$

$\Delta Gf° = -32.192 + 0.732\times10^{-3}T\ln T + 0.072\times10^{-6}T^{2} + 76.325T^{-1} - 6.981\times10^{-3}T$

Source: Data from Gurvich (196) who estimated most molecular constants.

GaP(c)
Gallium Phosphide
[Formation: $Ga(c,l) + P(c,l,1/4P_4(g)) = GaP(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.542	12.280	12.280	0	-28.100	-25.924	19.003
300	10.560	12.345	12.280	.020	-28.103	-25.911	18.876
302.9	10.580	12.447	12.279	.051	-28.108	-25.890	18.680
302.9	10.580	12.447	12.279	.051	-29.444	-25.890	18.680
317.3	10.680	12.940	12.298	.204	-29.471	-25.720	17.715
317.3	10.680	12.940	12.298	.204	-29.628	-25.720	17.715
400	11.251	15.490	12.705	1.114	-29.780	-24.682	13.485
500	11.613	18.043	13.525	2.259	-29.908	-23.390	10.224
550	11.729	19.157	13.987	2.844	-29.958	-22.750	9.040
550	11.729	19.157	13.987	2.844	-32.866	-22.750	9.040
600	11.846	20.183	14.461	3.433	-32.829	-21.832	7.952
700	12.018	22.022	15.413	4.626	-32.744	-20.005	6.246
800	12.158	23.636	16.341	5.836	-32.647	-18.190	4.969
900	12.279	25.076	17.235	7.057	-32.543	-16.391	3.980
1000	12.388	26.375	18.084	8.291	-32.429	-14.601	3.191
1100*	12.489	27.560	18.892	9.535	-32.307	-12.824	2.548
1200	12.585	28.651	19.661	10.788	-32.178	-11.060	2.014
1300	12.677	29.662	20.391	12.052	-32.039	-9.305	1.564
1400	12.767	30.605	21.088	13.324	-31.893	-7.562	1.181
1500	12.855	31.489	21.752	14.605	-31.739	-5.831	.850

*Data extrapolated above 1100 K.

Phase changes:
302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.
317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.
1730 K, melting point of GaP; ΔH° = 29.58 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K:
$Cp° = 11.719 + 0.794x10^{-3}T - 1.257x10^{5}T^{-2}$
$H°-H°_{298} = 11.719x10^{-3}T + 0.397x10^{-6}T^{2} + 1.257x10^{2}T^{-1} - 3.951$

Formation equations (kcal/mol):

298.15-302.9 K:
$ΔHf° = -28.689 + 1.424x10^{-3}T - 2.888x10^{-6}T^{2} + 125.700T^{-1}$
$ΔGf° = -28.689 - 1.424x10^{-3}TlnT + 2.888x10^{-6}T^{2} + 62.850T^{-1} + 15.820x10^{-3}T$

302.9-317.3 K:
$ΔHf° = -30.395 + 1.920x10^{-3}T - 2.914x10^{-6}T^{2} + 192.900T^{-1}$
$ΔGf° = -30.395 - 1.920x10^{-3}TlnT + 2.914x10^{-6}T^{2} + 96.450T^{-1} + 23.911x10^{-3}T$

317.3-550 K:
$ΔHf° = -30.082 - 0.573x10^{-3}T + 0.271x10^{-6}T^{2} + 192.900T^{-1}$
$ΔGf° = -30.082 + 0.573x10^{-3}TlnT - 0.271x10^{-6}T^{2} + 96.450T^{-1} + 9.575x10^{-3}T$

550-1500 K:
$ΔHf° = -33.542 + 0.765x10^{-3}T + 0.267x10^{-6}T^{2} + 92.600T^{-1}$
$ΔGf° = -33.542 - 0.765x10^{-3}TlnT - 0.267x10^{-6}T^{2} + 46.300T^{-1} + 24.473x10^{-3}T$

Sources: Enthalpy of formation at 298 K and fusion data from Tmar (492). Low-temperature heat capacities and entropy at 298 K from Koshchenko (280). High-temperature data based on Pankratz (381).

GaSb(c,l)
Gallium Antimonide
[Formation: Ga(c,l) + Sb(c,l) = GaSb(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.600	18.180	18.180	0	-10.000	-9.267	6.793
300	11.606	18.252	18.180	.022	-10.001	-9.261	6.747
302.9	11.615	18.364	18.180	.056	-10.004	-9.255	6.678
302.9	11.615	18.364	18.180	.056	-11.340	-9.255	6.678
400	11.922	21.634	18.639	1.198	-11.432	-8.572	4.683
500	12.214	24.326	19.514	2.406	-11.495	-7.846	3.429
600	12.500	26.578	20.511	3.640	-11.540	-7.117	2.592
700	12.780	28.526	21.520	4.904	-11.571	-6.374	1.990
800	13.058	30.252	22.507	6.196	-11.600	-5.635	1.539
900	13.336	31.806	23.455	7.516	-11.635	-4.885	1.186
903.9	13.347	31.864	23.491	7.568	-11.637	-4.856	1.174
903.9	13.347	31.864	23.491	7.568	-16.387	-4.856	1.174
985	13.570	33.020	24.228	8.660	-16.417	-3.823	.848
985	15.000	48.816	24.228	24.220	-.857	-3.823	.848
1000	15.000	49.044	24.600	24.444	-.841	-3.870	.846
1100	15.000	50.472	26.887	25.944	-.726	-4.171	.829
1200	15.000	51.778	28.908	27.444	-.611	-4.494	.818

Phase changes: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.
903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.
985 K, melting point of GaSb; ΔH° = 15.560 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-985 K: $Cp° = 10.874 + 2.746\times10^{-3}T - 0.080\times10^{5}T^{-2}$
$H° - H°_{298} = 10.874\times10^{-3}T + 1.373\times10^{-6}T^{2} + 0.080\times10^{2}T^{-1} - 3.391$
985-1200 K: $Cp° = 15.000$
$H° - H°_{298} = 15.000\times10^{-3}T + 9.445$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = -9.897 - 0.710\times10^{-3}T + 0.101\times10^{-6}T^{2} + 29.600T^{-1}$
$\Delta Gf° = -9.897 + 0.710\times10^{-3}T\ln T - 0.101\times10^{-6}T^{2} + 14.800T^{-1} - 2.071\times10^{-3}T$
302.9-903.9 K: $\Delta Hf° = -11.602 - 0.214\times10^{-3}T + 0.075\times10^{-6}T^{2} + 96.800T^{-1}$
$\Delta Gf° = -11.602 + 0.214\times10^{-3}T\ln T - 0.075\times10^{-6}T^{2} + 48.400T^{-1} + 6.020\times10^{-3}T$
903.9-985 K: $\Delta Hf° = -15.106 - 2.626\times10^{-3}T + 1.247\times10^{-6}T^{2} + 75.200T^{-1}$
$\Delta Gf° = -15.106 + 2.626\times10^{-3}T\ln T - 1.247\times10^{-6}T^{2} + 37.600T^{-1} - 5.449\times10^{-3}T$
985-1200 K: $\Delta Hf° = -2.270 + 1.500\times10^{-3}T - 0.126\times10^{-6}T^{2} + 67.200T^{-1}$
$\Delta Gf° = -2.270 - 1.500\times10^{-3}T\ln T + 0.126\times10^{-6}T^{2} + 33.600T^{-1} + 8.610\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from Piesbergen (400). High-temperature data based on Lichter (308).

$GaSe(c)$
Gallium Selenide
[Reaction: $Ga(c,l) + 0.5Se_2(g) = GaSe(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	11.590	16.800	16.800	0	-54.650	-48.073	35.238
300*	11.600	16.870	16.800	.021	-54.650	-48.033	34.991
302.9	11.609	16.982	16.801	.055	-54.650	-47.970	34.611
302.9	11.609	16.982	16.801	.055	-55.986	-47.970	34.611
400	11.910	20.250	17.257	1.197	-55.967	-45.401	24.805
500	12.220	22.940	18.132	2.404	-55.908	-42.763	18.691
600	12.530	25.200	19.132	3.641	-55.815	-40.147	14.623
700	12.840	27.150	20.136	4.910	-55.687	-37.539	11.720
800	13.150	28.890	21.129	6.209	-55.527	-34.961	9.551
900	13.460	30.450	22.072	7.540	-55.333	-32.396	7.867
1000	13.770	31.890	22.989	8.901	-55.107	-29.867	6.527
1100	14.080	33.210	23.852	10.294	-54.846	-27.345	5.433
1200	14.390	34.450	24.686	11.717	-54.552	-24.861	4.528

*Data above 298 K estimated.

Phase change: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 10.670 + 3.100\times10^{-3}T$

$H^\circ - H^\circ_{298} = 10.670\times10^{-3}T + 1.550\times10^{-6}T^2 - 3.319$

Reaction equations (kcal/mol):

298.15-302.9 K: $\Delta Hr^\circ = -54.347 - 1.158\times10^{-3}T + 1.610\times10^{-6}T^2 - 29.950T^{-1}$

$\Delta Gr^\circ = -54.347 + 1.158\times10^{-3}T\ln T - 1.610\times10^{-6}T^2 - 14.975T^{-1} + 15.093\times10^{-3}T$

302.9-1200 K: $\Delta Hr^\circ = -56.053 - 0.662\times10^{-3}T + 1.584\times10^{-6}T^2 + 37.250T^{-1}$

$\Delta Gr^\circ = -56.053 + 0.662\times10^{-3}T\ln T - 1.584\times10^{-6}T^2 + 18.625T^{-1} + 23.184\times10^{-3}T$

Source: Data from Mills (332) who estimated all above 298 K.

$Ga_2Se_3(c)$
Digallium Triselenide
[Reaction: $2Ga(c,l) + 1.5Se_2(g) = Ga_2Se_3(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	27.790	43.000	43.000	0	-147.650	-128.623	94.282
300*	27.800	43.170	43.000	.052	-147.649	-128.505	93.614
302.9	27.825	43.438	43.000	.133	-147.649	-128.321	92.586
302.9	27.825	43.438	43.000	.133	-150.321	-128.321	92.586
400	28.650	51.290	44.105	2.874	-150.309	-121.269	66.258
500	29.490	57.770	46.208	5.781	-150.202	-114.016	49.836
600	30.330	63.220	48.600	8.772	-150.006	-106.798	38.901
700	31.180	67.960	51.034	11.848	-149.717	-99.614	31.101
800	32.020	72.180	53.420	15.008	-149.339	-92.478	25.264
900	32.870	76.000	55.720	18.252	-148.871	-85.401	20.738
1000	33.710	79.500	57.919	21.581	-148.311	-78.376	17.129
1100	34.550	82.760	60.038	24.994	-147.659	-71.418	14.189
1200	35.400	85.800	62.057	28.492	-146.913	-64.516	11.750
1300	36.240	88.670	63.998	32.074	-146.075	-57.679	9.697

*Data above 298 K estimated except temperature and enthalpy of fusion.

Phase changes: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.
1280 K, melting point of Ga_2Se_3; ΔH° = 20.1 ± 1.7 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 25.270 + 8.440\text{x}10^{-3}T$
$H^\circ - H^\circ_{298} = 25.270\text{x}10^{-3}T + 4.220\text{x}10^{-6}T^2 - 7.909$

Reaction equations (kcal/mol):

298.15-302.9 K: $\Delta Hr^\circ = -146.640 - 3.718\text{x}10^{-3}T + 4.498\text{x}10^{-6}T^2 - 89.850T^{-1}$
$\Delta Gr^\circ = -146.640 + 3.718\text{x}10^{-3}T\ln T - 4.498\text{x}10^{-6}T^2 - 44.925T^{-1} + 41.091\text{x}10^{-3}T$
302.9-1300 K: $\Delta Hr^\circ = -150.051 - 2.726\text{x}10^{-3}T + 4.446\text{x}10^{-6}T^2 + 44.550T^{-1}$
$\Delta Gr^\circ = -150.051 + 2.726\text{x}10^{-3}T\ln T - 4.446\text{x}10^{-6}T^2 + 22.275T^{-1} + 57.273\text{x}10^{-3}T$

Sources: Data from Mills (332) who estimated all above 298 K except temperature and enthalpy of fusion.

$GaTe(c,l)$
Gallium Telluride
[Reaction: $Ga(c,l) + 0.5Te_2(g) = GaTe(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	11.813	20.410	20.410	0	-97.965	-91.918	67.377
300*	11.831	20.483	20.410	.022	-97.963	-91.881	66.934
302.9	11.854	20.597	20.411	.056	-97.960	-91.823	66.251
302.9	11.854	20.597	20.411	.056	-99.296	-91.823	66.251
400	12.619	24.003	20.885	1.247	-99.173	-89.442	48.868
500	13.178	26.882	21.806	2.538	-98.974	-87.030	38.040
600	13.646	29.327	22.860	3.880	-98.727	-84.662	30.838
700	14.073	31.463	23.940	5.266	-98.442	-82.340	25.707
800	14.476	33.368	25.000	6.694	-98.122	-80.062	21.872
900	14.867	35.096	26.028	8.161	-97.770	-77.826	18.898
1000	15.249	36.682	27.015	9.667	-97.388	-75.630	16.529
1100	15.626	38.153	27.961	11.211	-96.976	-73.472	14.597
1107	15.652	38.253	28.027	11.320	-96.946	-73.324	14.476
1107	41.000	46.726	28.027	20.700	-87.566	-73.324	14.476
1200	41.000	50.033	29.606	24.513	-84.814	-72.239	13.156
1300	41.000	53.315	31.305	28.613	-81.861	-71.310	11.988

*Data extrapolated 300 to 1095 K.

Phase changes: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.
1107 K, melting point of GaTe; ΔH° = 9.380 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1107 K: $Cp° = 11.719 + 3.618\text{x}10^{-3}T - 0.876\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 11.719\text{x}10^{-3}T + 1.809\text{x}10^{-6}T^{2} + 0.876\text{x}10^{2}T^{-1} - 3.949$
1107-1300 K: $Cp° = 41.000$
$H°-H°_{298} = 41.000\text{x}10^{-3}T - 24.687$

Reaction equations (kcal/mol):

298.15-302.9 K: $\Delta Hr° = -98.619 + 0.923\text{x}10^{-3}T + 1.413\text{x}10^{-6}T^{2} + 75.500T^{-1}$
$\Delta Gr° = -98.619 - 0.923\text{x}10^{-3}T\ln T - 1.413\text{x}10^{-6}T^{2} + 37.750T^{-1} + 27.735\text{x}10^{-3}T$
302.9-1107 K: $\Delta Hr° = -100.325 + 1.419\text{x}10^{-3}T + 1.387\text{x}10^{-6}T^{2} + 142.700T^{-1}$
$\Delta Gr° = -100.325 - 1.419\text{x}10^{-3}T\ln T - 1.387\text{x}10^{-6}T^{2} + 71.350T^{-1} + 35.826\text{x}10^{-3}T$
1107-1300 K: $\Delta Hr° = -121.063 + 30.701\text{x}10^{-3}T - 0.422\text{x}10^{-6}T^{2} + 55.100T^{-1}$
$\Delta Gr° = -121.063 - 30.701\text{x}10^{-3}T\ln T + 0.422\text{x}10^{-6}T^{2} + 27.550T^{-1} + 257.836\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Said (432). Low-temperature heat capacities and entropy at 298 K from Kerimov (252). High-temperature data based on Said (432).

GdO(g)
Gadolinium Monoxide (ideal gas)
[Formation: $Gd(c,l) + 0.5O_2(g) = GdO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	7.560	60.539	60.539	0	-16.500	-22.402	16.421
300	7.560	60.587	60.540	.014	-16.508	-22.440	16.347
400	7.940	62.816	60.841	.790	-16.825	-24.369	13.314
500	8.210	64.618	61.422	1.598	-17.055	-26.229	11.464
600	8.390	66.132	62.084	2.429	-17.288	-28.030	10.210
700	8.520	67.437	62.758	3.275	-17.537	-29.800	9.304
800	8.610	68.580	63.416	4.131	-17.807	-31.535	8.615
900	8.670	69.598	64.047	4.996	-18.096	-33.232	8.070
1000	8.720	70.514	64.649	5.865	-18.407	-34.906	7.629
1100	8.750	71.347	65.221	6.739	-18.740	-36.529	7.257
1200	8.780	72.111	65.764	7.616	-19.099	-38.139	6.946
1300	8.800	72.814	66.279	8.495	-19.486	-39.710	6.676
1400	8.820	73.468	66.770	9.377	-19.903	-41.241	6.438
1500	8.840	74.077	67.237	10.260	-20.352	-42.747	6.228
1533	8.843	74.269	67.386	10.552	-20.509	-43.240	6.164
1533	8.843	74.269	67.386	10.552	-21.444	-43.240	6.164
1585	8.849	74.565	67.617	11.012	-21.567	-43.986	6.065
1585	8.849	74.565	67.617	11.012	-23.970	-43.986	6.065
1600	8.850	74.648	67.682	11.145	-24.036	-44.178	6.034
1700	8.860	75.184	68.108	12.030	-24.480	-45.419	5.839
1800	8.870	75.692	68.516	12.917	-24.925	-46.635	5.662
1900	8.880	76.171	68.906	13.804	-25.373	-47.828	5.501
2000	8.880	76.627	69.281	14.692	-25.823	-49.010	5.356

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1533 K, α - β transition point of Gd; ΔH° = 0.935 kcal/mol.
1585 K, melting point of Gd; ΔH° = 2.403 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.437 + 0.310\times10^{-3}T - 0.861\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.437\times10^{-3}T + 0.155\times10^{-6}T^2 + 0.861\times10^{2}T^{-1} - 2.818$

Formation equations (kcal/mol):

298.15-1533 K: $\Delta Hf^\circ = -18.535 + 2.036\times10^{-3}T - 2.300\times10^{-6}T^2 + 486.600T^{-1}$

$\Delta Gf^\circ = -18.535 - 2.036\times10^{-3}T\ln T + 2.300\times10^{-6}T^2 + 243.300T^{-1} - 4.794\times10^{-3}T$

1533-1585 K: $\Delta Hf^\circ = -18.176 - 2.005\times10^{-3}T - 0.096\times10^{-6}T^2 + 63.500T^{-1}$

$\Delta Gf^\circ = -18.176 + 2.005\times10^{-3}T\ln T + 0.096\times10^{-6}T^2 + 31.750T^{-1} - 31.202\times10^{-3}T$

1585-2000 K: $\Delta Hf^\circ = -17.325 - 4.058\times10^{-3}T - 0.096\times10^{-6}T^2 + 63.500T^{-1}$

$\Delta Gf^\circ = -17.325 + 4.058\times10^{-3}T\ln T + 0.096\times10^{-6}T^2 + 31.750T^{-1} - 46.866\times10^{-3}T$

Source: Data from Pedley (396) who estimated all except enthalpy of formation at 298 K.

GdP(c)
Gadolinium Phosphide
[Formation: Gd(c,l) + P(c,l,1/4P_4(g)) = GdP(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	11.611	19.570	19.570	0	-75.000	-73.065	53.557
300	11.622	19.642	19.572	.021	-75.006	-73.055	53.220
317.3	11.700	20.296	19.594	.223	-75.053	-72.940	50.239
317.3	11.700	20.296	19.594	.223	-75.210	-72.940	50.239
400	12.070	23.053	20.033	1.208	-75.332	-72.337	39.522
500	12.347	25.778	20.918	2.430	-75.412	-71.579	31.287
550	12.453	26.961	21.414	3.051	-75.447	-71.197	28.291
550	12.453	26.961	21.414	3.051	-78.355	-71.197	28.291
600	12.558	28.049	21.922	3.676	-78.308	-70.548	25.697
700	12.736	29.998	22.939	4.941	-78.221	-69.259	21.623
800	12.898	31.709	23.931	6.222	-78.145	-67.985	18.572
900	13.051	33.238	24.882	7.520	-78.076	-66.719	16.201
1000	13.197	34.620	25.788	8.832	-78.016	-65.468	14.308
1100	13.339	35.885	26.650	10.159	-77.963	-64.205	12.756
1200	13.478	37.051	27.468	11.500	-77.923	-62.964	11.467
1300	13.616	38.136	28.248	12.855	-77.896	-61.720	10.376
1400	13.752	39.150	28.991	14.223	-77.886	-60.466	9.439
1500	13.887	40.103	29.700	15.605	-77.893	-59.220	8.628
1533	13.932	40.406	29.927	16.064	-77.901	-58.810	8.384
1533	13.932	40.406	29.927	16.064	-78.836	-58.810	8.384
1585	14.002	40.872	30.278	16.791	-78.720	-58.141	8.017
1585	14.002	40.872	30.278	16.791	-81.123	-58.141	8.017
1600	14.022	41.004	30.378	17.001	-81.120	-57.926	7.912
1700	14.155	41.858	31.029	18.409	-81.093	-56.475	7.260
1800	14.289	42.670	31.652	19.832	-81.051	-55.021	6.680
1900	14.422	43.447	32.254	21.267	-80.998	-53.579	6.163
2000	14.554	44.190	32.832	22.716	-80.930	-52.148	5.698

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P; ΔH° = 2.908 kcal/mol of P.
1533 K, α - β transition point of Gd; ΔH° = 0.935 kcal/mol.
1585 K, melting point of Gd; ΔH° = 2.403 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2400 K: $Cp^\circ = 11.954 + 1.308\text{x}10^{-3}T - 0.651\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 11.954\text{x}10^{-3}T + 0.654\text{x}10^{-6}T^2 + 0.651\text{x}10^{2}T^{-1} - 3.841$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf^\circ = -77.817 + 5.369\text{x}10^{-3}T - 4.734\text{x}10^{-6}T^2 + 488.200T^{-1}$
$\Delta Gf^\circ = -77.817 - 5.369\text{x}10^{-3}T\ln T + 4.734\text{x}10^{-6}T^2 + 244.100T^{-1} + 42.372\text{x}10^{-3}T$
317.3-550 K: $\Delta Hf^\circ = -77.504 + 2.876\text{x}10^{-3}T - 1.549\text{x}10^{-6}T^2 + 488.200T^{-1}$
$\Delta Gf^\circ = -77.504 - 2.876\text{x}10^{-3}T\ln T + 1.549\text{x}10^{-6}T^2 + 244.100T^{-1} + 28.036\text{x}10^{-3}T$
550-1533 K: $\Delta Hf^\circ = -80.964 + 4.214\text{x}10^{-3}T - 1.553\text{x}10^{-6}T^2 + 387.900T^{-1}$
$\Delta Gf^\circ = -80.964 - 4.214\text{x}10^{-3}T\ln T + 1.553\text{x}10^{-6}T^2 + 193.950T^{-1} + 42.934\text{x}10^{-3}T$
1533-1585 K: $\Delta Hf^\circ = -80.606 + 0.173\text{x}10^{-3}T + 0.650\text{x}10^{-6}T^2 - 35.200T^{-1}$
$\Delta Gf^\circ = -80.606 - 0.173\text{x}10^{-3}T\ln T - 0.650\text{x}10^{-6}T^2 - 17.600T^{-1} + 16.527\text{x}10^{-3}T$
1585-2000 K: $\Delta Hf^\circ = -79.755 - 1.880\text{x}10^{-3}T + 0.650\text{x}10^{-6}T^2 - 35.200T^{-1}$
$\Delta Gf^\circ = -79.755 + 1.880\text{x}10^{-3}T\ln T - 0.650\text{x}10^{-6}T^2 - 17.600T^{-1} + 0.862\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K and high-temperature data from Gordienko (179). Low-temperature heat capacities and entropy at 298 K from Rakhmenkulov (413).

$GeAs(c,l)$
Germanium Arsenide
[Formation: $Ge(c) + As[a,1/4As_4(g)] = GeAs(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.408	15.730	15.730	0	-20.000	-19.930	14.609
300	11.417	15.800	15.730	.021	-20.000	-19.931	14.520
400	11.864	19.143	16.183	1.184	-20.012	-19.907	10.877
500	12.327	21.841	17.053	2.394	-20.005	-19.879	8.689
600	12.788	24.129	18.046	3.650	-19.976	-19.852	7.231
700	13.249	26.135	19.062	4.951	-19.922	-19.840	6.194
800	13.708	27.934	20.060	6.299	-19.841	-19.833	5.418
876	14.058	29.194	20.798	7.354	-19.765	-19.835	4.948
876	14.058	29.194	20.798	7.354	-28.074	-19.835	4.948
900	14.168	29.575	21.027	7.693	-28.005	-19.610	4.762
1000	14.627	31.092	21.959	9.133	-27.700	-18.700	4.087
1025	14.742	31.454	22.186	9.500	-27.619	-18.476	3.939
1025	21.000	46.371	22.186	24.790	-12.329	-18.476	3.939
1100	21.000	47.854	23.886	26.365	-11.621	-18.948	3.765

Phase changes: 876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol $As_4(g)$.
1025 K, melting point of GeAs; ΔH° = 15.290 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1025 K: $Cp° = 9.989 + 4.642x10^{-3}T + 0.031x10^{5}T^{-2}$
$H°- H°_{298} = 9.989x10^{-3}T + 2.321x10^{-6}T^{2} - 0.031x10^{2}T^{-1} - 3.174$
1025-1100 K: $Cp° = 21.000$
$H°- H°_{298} = 21.000x10^{-3}T + 3.265$

Formation equations (kcal/mol):

298.15-876 K: $ΔHf° = -19.596 - 1.283x10^{-3}T + 1.284x10^{-6}T^{2} - 40.400T^{-1}$
$ΔGf° = -19.596 + 1.283x10^{-3}TlnT - 1.284x10^{-6}T^{2} - 20.200T^{-1} - 7.821x10^{-3}T$
876-1025 K: $ΔHf° = -28.924 - 0.585x10^{-3}T + 1.862x10^{-6}T^{2} - 71.900T^{-1}$
$ΔGf° = -28.924 + 0.585x10^{-3}TlnT - 1.862x10^{-6}T^{2} - 35.950T^{-1} + 8.084x10^{-3}T$
1025-1100 K: $ΔHf° = -22.485 + 10.426x10^{-3}T - 0.459x10^{-6}T^{2} - 68.800T^{-1}$
$ΔGf° = -22.485 - 10.426x10^{-3}TlnT + 0.459x10^{-6}T^{2} - 34.400T^{-1} + 75.754x10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Ferro (149). Low-temperature heat capacities and entropy at 298 K from Koshchenko (280). High-temperature data based on Blachnik (46).

GeO(g)
Germanium Monoxide (ideal gas)
[Formation: Ge(c,l) + 0.5O_2(g) = GeO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.340	53.485	53.485	0	-8.500	-14.926	10.941
300	7.350	53.533	53.486	.014	-8.503	-14.967	10.903
400	7.740	55.702	53.779	.769	-8.677	-17.096	9.341
500	8.040	57.463	54.345	1.559	-8.843	-19.179	8.383
600	8.260	58.949	54.992	2.374	-9.005	-21.228	7.732
700	8.410	60.234	55.651	3.208	-9.168	-23.256	7.261
800	8.530	61.365	56.296	4.055	-9.334	-25.258	6.900
900	8.620	62.376	56.917	4.913	-9.509	-27.235	6.614
1000	8.680	63.287	57.509	5.778	-9.699	-29.201	6.382
1100	8.740	64.117	58.072	6.649	-9.906	-31.139	6.187
1200	8.780	64.879	58.608	7.525	-10.131	-33.056	6.020
1210.4	8.783	64.955	58.662	7.616	-10.155	-33.251	6.004
1210.4	8.783	64.955	58.662	7.616	-18.985	-33.251	6.004
1300	8.810	65.583	59.118	8.405	-19.170	-34.297	5.766
1400	8.840	66.238	59.604	9.288	-19.378	-35.453	5.534
1500	8.870	66.849	60.067	10.173	-19.588	-36.587	5.331
1600	8.890	67.422	60.509	11.061	-19.799	-37.723	5.153
1700	8.910	67.961	60.931	11.951	-20.010	-38.836	4.993
1800	8.920	68.471	61.336	12.843	-20.222	-39.932	4.848
1900	8.940	68.954	61.725	13.736	-20.436	-41.016	4.718
2000	8.950	69.414	62.099	14.631	-20.651	-42.093	4.600

Phase change: 1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.204 + 0.492\text{x}10^{-3}T - 0.898\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.204\text{x}10^{-3}T + 0.246\text{x}10^{-6}T^{2} + 0.898\text{x}10^{2}T^{-1} - 2.769$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf^\circ = -8.304 - 0.992\text{x}10^{-3}T - 0.471\text{x}10^{-6}T^{2} + 42.300T^{-1}$

$\Delta Gf^\circ = -8.304 + 0.992\text{x}10^{-3}T\ln T + 0.471\text{x}10^{-6}T^{2} + 21.150T^{-1} - 28.240\text{x}10^{-3}T$

1210.4-2000 K: $\Delta Hf^\circ = -16.604 - 2.011\text{x}10^{-3}T - 0.005\text{x}10^{-6}T^{2} + 67.200T^{-1}$

$\Delta Gf^\circ = -16.604 + 2.011\text{x}10^{-3}T\ln T + 0.005\text{x}10^{-6}T^{2} + 33.600T^{-1} - 28.061\text{x}10^{-3}T$

Source: Data from Pedley (396).

GeSe(g)
Germanium Selenide (ideal gas)
[Reaction: Ge(c,l) + 0.5Se_2(g) = GeSe(g)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	8.380	59.200	59.200	0	8.550	1.791	-1.313
300	8.390	59.250	59.200	.016	8.547	1.749	-1.274
400	8.590	61.700	59.533	.867	8.326	-.486	.266
500	8.690	63.630	60.168	1.731	8.096	-2.662	1.164
600	8.750	65.220	60.880	2.604	7.863	-4.788	1.744
700	8.780	66.570	61.599	3.480	7.627	-6.881	2.148
800	8.810	67.750	62.300	4.360	7.389	-8.939	2.442
900	8.820	68.780	62.957	5.241	7.142	-10.957	2.661
1000	8.840	69.710	63.586	6.124	6.884	-12.962	2.833
1100	8.850	70.560	64.188	7.009	6.612	-14.936	2.968
1200	8.860	71.330	64.752	7.894	6.328	-16.880	3.074
1210.4	8.861	71.406	64.809	7.986	6.297	-17.077	3.083
1210.4	8.861	71.406	64.809	7.986	-2.533	-17.077	3.083
1300	8.870	72.040	65.285	8.781	-2.768	-18.140	3.050
1400	8.870	72.690	65.784	9.668	-3.029	-19.305	3.014
1500	8.880	73.310	66.273	10.555	-3.288	-20.463	2.981
1600	8.890	73.880	66.728	11.444	-3.542	-21.605	2.951
1700	8.890	74.420	67.165	12.333	-3.792	-22.721	2.921
1800	8.900	74.930	67.584	13.223	-4.039	-23.830	2.893
1900	8.900	75.410	67.982	14.113	-4.282	-24.916	2.866
2000	8.910	75.870	68.368	15.003	-4.522	-26.002	2.841

Phase change: 1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.841 + 0.040\times10^{-3}T - 0.420\times10^{5}T^{-2}$

$H°- H°_{298} = 8.841\times10^{-3}T + 0.020\times10^{-6}T^{2} + 0.420\times10^{2}T^{-1} - 2.779$

Reaction equations (kcal/mol):

298.15-1210.4 K: $\Delta Hr° = 9.236 - 2.072\times10^{-3}T - 0.287\times10^{-6}T^{2} - 12.850T^{-1}$

$\Delta Gr° = 9.236 + 2.072\times10^{-3}T\ln T + 0.287\times10^{-6}T^{2} - 6.425T^{-1} - 36.791\times10^{-3}T$

1210.4-2000 K: $\Delta Hr° = 0.936 - 3.091\times10^{-3}T + 0.179\times10^{-6}T^{2} + 12.050T^{-1}$

$\Delta Gr° = 0.936 + 3.091\times10^{-3}T\ln T - 0.179\times10^{-6}T^{2} + 6.025T^{-1} - 36.611\times10^{-3}T$

Source: Data from Mills (332).

$GeSe_2(c)$
Germanium Diselenide
[Reaction: $Ge(c) + Se_2(g) = GeSe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	17.010	26.900	26.900	0	-61.500	-49.953	36.616
300*	17.020	27.010	26.907	.031	-61.497	-49.884	36.340
400	17.680	31.990	27.575	1.766	-61.332	-46.036	25.153
500	18.340	36.010	28.874	3.568	-61.128	-42.233	18.460
600	19.010	39.410	30.352	5.435	-60.872	-38.474	14.014
700	19.670	42.390	31.863	7.369	-60.555	-34.767	10.855
800	20.330	45.060	33.348	9.370	-60.176	-31.104	8.497
900	21.000	47.500	34.793	11.436	-59.740	-27.502	6.678
1000	21.660	49.740	36.171	13.569	-59.248	-23.948	5.234
1012	21.740	50.000	36.335	13.829	-59.186	-23.526	5.081

*Data above 298 K estimated.

Phase change: 1012 K, melting point of $GeSe_2$; ΔH° = 6.3 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1012 K: $Cp^\circ = 15.030 + 6.630\times10^{-3}T$

$H^\circ - H^\circ_{298} = 15.030\times10^{-3}T + 3.315\times10^{-6}T^2 - 4.776$

Reaction equations (kcal/mol):

298.15-1012 K: $\Delta Hr^\circ = -61.135 - 1.215\times10^{-3}T + 3.168\times10^{-6}T^2 - 84.800T^{-1}$

$\Delta Gr^\circ = -61.135 + 1.215\times10^{-3}T\ln T - 3.168\times10^{-6}T^2 - 42.400T^{-1} + 32.005\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Irene (214), Karbanov (236), and Zlomanov (547). Other data from Mills (332) who estimated all above 298 K.

GeTe(c,l)
Germanium Telluride
[Reaction: $Ge(c,l) + 0.5Te_2(g) = GeTe(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	12.400	21.250	21.250	0	-30.765	-25.662	18.811
300	12.410	21.330	21.250	.025	-30.758	-25.631	18.672
400	12.910	24.970	21.745	1.290	-30.508	-23.962	13.092
500	13.690	27.920	22.690	2.615	-30.221	-22.353	9.770
600	14.930	30.520	23.787	4.040	-29.852	-20.810	7.580
680	16.290	32.470	24.691	5.290	-29.458	-19.630	6.309
680	12.250	32.470	24.691	5.290	-29.458	-19.630	6.309
700	12.340	32.830	24.916	5.540	-29.424	-19.340	6.038
800	12.780	34.500	26.013	6.790	-29.261	-17.913	4.893
900	13.220	36.030	27.041	8.090	-29.067	-16.503	4.007
990	13.620	37.310	27.919	9.300	-28.874	-15.264	3.370
990	21.100	46.790	27.919	18.680	-19.494	-15.264	3.370
1000	21.020	47.000	28.110	18.890	-19.398	-15.223	3.327
1100	20.290	48.970	29.915	20.960	-18.484	-14.843	2.949
1200	19.550	50.700	31.575	22.950	-17.675	-14.543	2.649
1210.4	19.473	50.868	31.740	23.153	-17.596	-14.511	2.620
1210.4	19.473	50.868	31.740	23.153	-26.426	-14.511	2.620
1300	18.810	52.240	33.109	24.870	-25.758	-13.655	2.296

Phase changes: 680 K, α - β transition point of GeTe; ΔH° = 0 kcal/mol.
990 K, melting point of GeTe; ΔH° = 9.380 kcal/mol.
1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-680 K: $Cp^\circ = 6.385 + 13.482\times10^{-3}T + 1.774\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 6.385\times10^{-3}T + 6.741\times10^{-6}T^{2} - 1.774\times10^{2}T^{-1} - 1.908$
680-990 K: $Cp^\circ = 7.977 + 5.500\times10^{-3}T + 2.467\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 7.977\times10^{-3}T + 2.750\times10^{-6}T^{2} - 2.467\times10^{2}T^{-1} - 1.043$
990-1300 K: $Cp^\circ = 28.387 - 7.364\times10^{-3}T$
$H^\circ - H^\circ_{298} = 28.387\times10^{-3}T - 3.682\times10^{-6}T^{2} - 5.814$

Reaction equations (kcal/mol):

298.15-680 K: $\Delta Hr^\circ = -29.535 - 3.495\times10^{-3}T + 5.978\times10^{-6}T^{2} - 214.400T^{-1}$
$\Delta Gr^\circ = -29.535 + 3.495\times10^{-3}T\ln T - 5.978\times10^{-6}T^{2} - 107.200T^{-1} - 3.937\times10^{-3}T$
680-990 K: $\Delta Hr^\circ = -28.670 - 1.903\times10^{-3}T + 1.988\times10^{-6}T^{2} - 283.700T^{-1}$
$\Delta Gr^\circ = -28.670 + 1.903\times10^{-3}T\ln T - 1.988\times10^{-6}T^{2} - 141.850T^{-1} + 2.535\times10^{-3}T$
990-1210.4 K: $\Delta Hr^\circ = -33.441 + 18.506\times10^{-3}T - 4.444\times10^{-6}T^{2} - 37.000T^{-1}$
$\Delta Gr^\circ = -33.441 - 18.506\times10^{-3}T\ln T + 4.444\times10^{-6}T^{2} - 18.500T^{-1} + 141.643\times10^{-3}T$
1210.4-1300 K: $\Delta Hr^\circ = -41.741 + 17.487\times10^{-3}T - 3.978\times10^{-6}T^{2} - 12.100T^{-1}$
$\Delta Gr^\circ = -41.741 - 17.487\times10^{-3}T\ln T + 3.978\times10^{-6}T^{2} - 6.050T^{-1} + 141.822\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (332). Low-temperature heat capacities and entropy at 298 K from Zhdanov (544). High-temperature data based on Castanet (72).

$GeTe(g)$
Germanium Telluride (ideal gas)
[Reaction: $Ge(c,l) + 0.5Te_2(g) = GeTe(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	8.590	61.100	61.100	0	15.635	8.857	-6.492
300	8.600	61.150	61.100	.016	15.633	8.814	-6.421
400	8.740	63.650	61.438	.885	15.487	6.561	-3.585
500	8.810	65.610	62.084	1.763	15.327	4.350	-1.901
600	8.850	67.220	62.810	2.646	15.154	2.176	-.793
700	8.870	68.590	63.544	3.532	14.969	.020	-.006
800	8.880	69.770	64.246	4.419	14.768	-2.100	.574
900	8.890	70.820	64.922	5.308	14.551	-4.196	1.019
1000	8.900	71.760	65.562	6.198	14.310	-6.275	1.371
1100	8.910	72.610	66.166	7.088	14.044	-8.319	1.653
1200	8.910	73.380	66.731	7.979	13.754	-10.329	1.881
1210.4	8.910	73.457	66.788	8.072	13.723	-10.534	1.902
1210.4	8.910	73.457	66.788	8.072	4.893	-10.534	1.902
1300	8.910	74.090	67.267	8.870	4.642	-11.660	1.960
1400	8.910	74.750	67.778	9.761	4.352	-12.903	2.014
1500	8.920	75.370	68.268	10.653	4.062	-14.126	2.058
1600	8.920	75.950	68.735	11.544	3.771	-15.349	2.097
1700	8.920	76.490	69.175	12.436	3.482	-16.527	2.125
1800	8.920	77.000	69.596	13.328	3.194	-17.694	2.148
1900	8.920	77.480	69.996	14.220	2.909	-18.836	2.167
2000	8.920	77.940	70.383	15.113	2.627	-19.973	2.183

Phase change: 1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.935 - 0.002\text{x}10^{-3}T - 0.306\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 8.935\text{x}10^{-3}T - 0.001\text{x}10^{-6}T^{2} + 0.306\text{x}10^{2}T^{-1} - 2.767$

Reaction equations (kcal/mol):

298.15-1210.4 K: $\Delta Hr° = 16.006 - 0.945\text{x}10^{-3}T - 0.763\text{x}10^{-6}T^{2} - 6.400T^{-1}$

$\Delta Gr° = 16.006 + 0.945\text{x}10^{-3}T\ln T + 0.763\text{x}10^{-6}T^{2} - 3.200T^{-1} - 29.559\text{x}10^{-3}T$

1210.4-2000 K: $\Delta Hr° = 7.706 - 1.964\text{x}10^{-3}T - 0.297\text{x}10^{-6}T^{2} + 18.500T^{-1}$

$\Delta Gr° = 7.706 + 1.964\text{x}10^{-3}T\ln T + 0.297\text{x}10^{-6}T^{2} + 9.250T^{-1} - 29.380\text{x}10^{-3}T$

Source: Data from Mills (332).

HAlO(g)
Aluminum Oxide Hydride (ideal gas)
[Formation: $0.5H_2(g) + Al(c,l) + 0.5O_2(g) = HAlO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.262	51.464	51.464	0	8.000	6.634	-4.863
300	8.285	51.515	51.465	.015	7.991	6.625	-4.826
400	9.541	54.072	51.805	.907	7.583	6.234	-3.406
500	10.634	56.323	52.487	1.918	7.255	5.936	-2.595
600	11.495	58.341	53.298	3.026	6.984	5.700	-2.076
700	12.154	60.165	54.151	4.210	6.747	5.505	-1.719
800	12.656	61.822	55.007	5.452	6.518	5.343	-1.460
900	13.042	63.336	55.850	6.737	6.280	5.209	-1.265
933.61	13.143	63.816	56.129	7.177	6.196	5.170	-1.210
933.61	13.143	63.816	56.129	7.177	3.616	5.170	-1.210
1000	13.342	64.726	56.669	8.057	3.478	5.286	-1.155
1100	13.578	66.009	57.460	9.404	3.283	5.476	-1.088
1200	13.767	67.199	58.223	10.771	3.099	5.684	-1.035
1300	13.919	68.307	58.956	12.156	2.924	5.907	-.993
1400	14.043	69.344	59.663	13.554	2.753	6.142	-.959
1500	14.146	70.316	60.340	14.964	2.586	6.390	-.931
1600	14.232	71.232	60.993	16.383	2.418	6.648	-.908
1700	14.304	72.097	61.621	17.810	2.252	6.919	-.889
1800	14.366	72.916	62.225	19.243	2.083	7.198	-.874
1900	14.418	73.695	62.809	20.683	1.915	7.487	-.861
2000	14.464	74.435	63.371	22.127	1.743	7.786	-.851

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.867 + 2.378\times10^{-3}T - 2.946\times10^{5}T^{-2}$

$H°-H°_{298} = 10.867\times10^{-3}T + 1.189\times10^{-6}T^{2} + 2.946\times10^{2}T^{-1} - 4.334$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = 7.260 - 0.568\times10^{-3}T - 0.999\times10^{-6}T^{2} + 297.650T^{-1}$

$\Delta Gf° = 7.260 + 0.568\times10^{-3}T\ln T + 0.999\times10^{-6}T^{2} + 148.825T^{-1} - 7.308\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = 5.992 - 3.566\times10^{-3}T + 0.728\times10^{-6}T^{2} + 280.250T^{-1}$

$\Delta Gf° = 5.992 + 3.566\times10^{-3}T\ln T - 0.728\times10^{-6}T^{2} + 140.125T^{-1} - 24.831\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$HBO_2(c,l)$
Metaboric Acid
[Formation: $0.5H_2(g) + B(\beta) + O_2(g) = HBO_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.075	11.711	11.711	0	-192.300	-176.108	129.089
300	13.101	11.792	11.712	.024	-192.301	-176.007	128.219
400	14.501	15.753	12.243	1.404	-192.294	-170.578	93.198
500	15.901	19.139	13.289	2.925	-192.261	-165.149	72.185
509	16.027	19.424	13.396	3.068	-192.257	-164.661	70.700
509	25.100	26.139	13.396	6.486	-188.839	-164.661	70.700
600	25.100	30.268	15.651	8.770	-187.996	-160.414	58.430
700	25.100	34.137	18.023	11.280	-187.133	-155.884	48.669
800	25.100	37.488	20.250	13.790	-186.320	-151.476	41.381
900	25.100	40.445	22.334	16.300	-185.549	-147.167	35.737
1000	25.100	43.089	24.279	18.810	-184.813	-142.942	31.239
1100	25.100	45.482	26.100	21.320	-184.109	-138.795	27.576
1200	25.100	47.666	27.808	23.830	-183.434	-134.703	24.533
1300	25.100	49.675	29.413	26.340	-182.787	-130.666	21.967
1400	25.100	51.535	30.928	28.850	-182.167	-126.680	19.775
1500	25.100	53.266	32.359	31.360	-181.573	-122.733	17.882

*Data except enthalpy of formation at 298 K and temperature and enthalpy of fusion estimated.

Phase change: 509 K, melting point of HBO_2; ΔH° = 3.418 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-509 K: $Cp° = 8.901 + 14.000\times10^{-3}T$

$H°-H°_{298} = 8.901\times10^{-3}T + 7.000\times10^{-6}T^2 - 3.276$

509-1500 K: $Cp° = 25.100$

$H°-H°_{298} = 25.100\times10^{-3}T - 6.290$

Formation equations (kcal/mol):

298.15-509 K: $\Delta Hf° = -190.058 - 6.280\times10^{-3}T + 5.595\times10^{-6}T^2 - 258.450T^{-1}$

$\Delta Gf° = -190.058 + 6.280\times10^{-3}T\ln T - 5.595\times10^{-6}T^2 - 129.225T^{-1} + 14.130\times10^{-3}T$

509-1500 K: $\Delta Hf° = -193.072 + 9.919\times10^{-3}T - 1.404\times10^{-6}T^2 - 258.450T^{-1}$

$\Delta Gf° = -193.072 - 9.919\times10^{-3}T\ln T + 1.404\times10^{-6}T^2 - 129.225T^{-1} + 117.447\times10^{-3}T$

Source: Data from Gurvich (196) who estimated all except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

$HBO_2(g)$
Metaboric Acid (ideal gas)
[Formation: $0.5H_2(g) + B(\beta) + O_2(g) = HBO_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.587	57.529	57.529	0	-134.610	-132.079	96.815
300	10.613	57.595	57.529	.020	-134.615	-132.062	96.206
400	11.938	60.835	57.962	1.149	-134.859	-131.176	71.670
500	13.022	63.620	58.822	2.399	-135.097	-130.225	56.921
600	13.899	66.074	59.829	3.747	-135.329	-129.231	47.072
700	14.617	68.272	60.881	5.174	-135.549	-128.195	40.024
800	15.216	70.265	61.932	6.666	-135.754	-127.131	34.730
900	15.723	72.087	62.960	8.214	-135.945	-126.041	30.607
1000	16.159	73.766	63.958	9.808	-136.124	-124.930	27.303
1100	16.536	75.325	64.921	11.444	-136.294	-123.808	24.598
1200	16.865	76.778	65.850	13.114	-136.460	-122.664	22.340
1300	17.154	78.140	66.744	14.815	-136.622	-121.505	20.427
1400	17.407	79.420	67.604	16.543	-136.784	-120.336	18.785
1500	17.630	80.629	68.432	18.296	-136.947	-119.152	17.360
1600	17.827	81.773	69.230	20.069	-137.118	-117.972	16.114
1700	18.002	82.859	70.000	21.860	-137.294	-116.768	15.011
1800	18.157	83.893	70.744	23.668	-137.479	-115.545	14.029
1900	18.295	84.878	71.462	25.491	-137.673	-114.319	13.149
2000	18.418	85.820	72.157	27.327	-137.877	-113.098	12.359

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.675 + 3.432x10^{-3}T - 2.765x10^{5}T^{-2}$
$H°-H°_{298} = 12.675x10^{-3}T + 1.716x10^{-6}T^{2} + 2.765x10^{2}T^{-1} - 4.859$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -133.951 - 2.506x10^{-3}T + 0.312x10^{-6}T^{2} + 18.050T^{-1}$
$\Delta Gf° = -133.951 + 2.506x10^{-3}TlnT - 0.312x10^{-6}T^{2} + 9.025T^{-1} - 8.007x10^{-3}T$

Source: Data from Gurvich (196).

H_3BO_3(c,l)
Boric Acid
[Formation: $1.5H_2(g) + B(\beta) + 1.5O_2(g) = H_3BO_3(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	19.442	21.210	21.210	0	-261.690	-231.721	169.854
300	19.541	21.331	21.211	.036	-261.698	-231.534	168.670
400	23.950	27.593	22.036	2.223	-261.934	-221.437	120.986
444.1	25.540	30.181	22.717	3.315	-261.952	-216.971	106.774
444.1	43.020	42.183	22.717	8.645	-256.622	-216.971	106.774
500	43.020	47.283	25.183	11.050	-255.659	-212.035	92.679
600	43.020	55.127	29.540	15.352	-254.014	-203.470	74.113
700	43.020	61.758	33.681	19.654	-252.451	-195.168	60.933
800	43.020	67.503	37.558	23.956	-250.951	-187.089	51.110

Phase change: 444.1 K, melting point of H_3PO_4; ΔH° = 5.330 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-444.1 K: $Cp° = 15.770 + 26.200\times10^{-3}T - 3.680\times10^{5}T^{-2}$
$H°-H°_{298} = 15.770\times10^{-3}T + 13.100\times10^{-6}T^{2} + 3.680\times10^{2}T^{-1} - 7.101$
444.1-800 K: $Cp° = 43.020$
$H°-H°_{298} = 43.020\times10^{-3}T - 10.460$

Formation equations (kcal/mol):

298.15-444.1 K: $\Delta Hf° = -260.190 - 9.482\times10^{-3}T + 11.025\times10^{-6}T^{2} + 103.450T^{-1}$
$\Delta Gf° = -260.190 + 9.482\times10^{-3}T\ln T - 11.025\times10^{-6}T^{2} + 51.725T^{-1} + 44.167\times10^{-3}T$
444.1-800 K: $\Delta Hf° = -263.549 + 17.768\times10^{-3}T - 2.075\times10^{-6}T^{2} - 264.550T^{-1}$
$\Delta Gf° = -263.549 - 17.768\times10^{-3}T\ln T + 2.075\times10^{-6}T^{2} - 132.275T^{-1} + 212.965\times10^{-3}T$

Source: Data from Gurvich (196).

$H_3BO_3(g)$
Boric Acid (ideal gas)
[Formation: $1.5H_2(g) + B(\beta) + 1.5O_2(g) = H_3BO_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	15.737	63.223	63.223	0	-240.440	-222.997	163.459
300	15.812	63.320	63.223	.029	-240.455	-222.887	162.371
400	19.423	68.384	63.889	1.798	-241.109	-216.928	118.523
500	22.204	73.031	65.259	3.886	-241.573	-210.823	92.150
600	24.321	77.275	66.913	6.217	-241.900	-204.643	74.540
700	25.966	81.153	68.676	8.734	-242.121	-198.415	61.947
800	27.292	84.709	70.459	11.400	-242.257	-192.159	52.495
900	28.397	87.990	72.229	14.185	-242.328	-185.894	45.141
1000	29.342	91.032	73.958	17.074	-242.344	-179.621	39.256
1100	30.163	93.868	75.641	20.050	-242.320	-173.355	34.442
1200	30.883	96.524	77.271	23.103	-242.262	-167.085	30.430
1300	31.518	99.021	78.849	26.224	-242.178	-160.819	27.036
1400	32.081	101.378	80.375	29.404	-242.076	-154.567	24.129
1500	32.580	103.609	81.850	32.638	-241.961	-148.317	21.609
1600	33.023	105.726	83.277	35.918	-241.840	-142.091	19.409
1700	33.418	107.740	84.657	39.241	-241.712	-135.856	17.465
1800	33.771	109.660	85.993	42.600	-241.587	-129.622	15.738
1900	34.086	111.495	87.288	45.994	-241.463	-123.404	14.195
2000	34.368	113.250	88.542	49.417	-241.345	-117.206	12.807

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.758 + 7.606\times10^{-3}T - 7.368\times10^{5}T^{-2}$

$H° - H°_{298} = 21.758\times10^{-3}T + 3.803\times10^{-6}T^{2} + 7.368\times10^{2}T^{-1} - 9.296$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -241.136 - 3.494\times10^{-3}T + 1.728\times10^{-6}T^{2} + 472.250T^{-1}$

$\Delta Gf° = -241.136 + 3.494\times10^{-3}T\ln T - 1.728\times10^{-6}T^{2} + 236.125T^{-1} + 38.790\times10^{-3}T$

Source: Data from Gurvich (196).

$HCN(g)$
Hydrogen Cyanide (ideal gas)
[Formation: $0.5H_2(g) + C(c) + 0.5N_2(g) = HCN(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	8.570	48.212	48.212	0	32.300	29.810	-21.851
300	8.587	48.265	48.212	.016	32.299	29.794	-21.705
400	9.376	50.849	48.559	.916	32.259	28.966	-15.826
500	9.974	53.008	49.238	1.885	32.210	28.148	-12.303
600	10.470	54.871	50.026	2.907	32.149	27.341	-9.959
700	10.909	56.519	50.839	3.976	32.080	26.544	-8.287
800	11.309	58.002	51.642	5.088	32.008	25.760	-7.037
900	11.674	59.355	52.425	6.237	31.935	24.982	-6.066
1000	12.005	60.603	53.182	7.421	31.866	24.212	-5.291
1100	12.305	61.761	53.909	8.637	31.801	23.461	-4.661
1200	12.574	62.843	54.609	9.881	31.739	22.695	-4.133
1300	12.815	63.860	55.282	11.151	31.680	21.944	-3.689
1400	13.031	64.817	55.929	12.443	31.625	21.197	-3.309
1500	13.224	65.723	56.552	13.756	31.571	20.454	-2.980
1600	13.396	66.582	57.153	15.087	31.522	19.714	-2.693
1700	13.551	67.399	57.731	16.435	31.473	18.977	-2.440
1800	13.689	68.177	58.290	17.797	31.425	18.245	-2.215
1900	13.813	68.921	58.830	19.172	31.379	17.513	-2.014
2000	13.925	69.632	59.353	20.559	31.332	16.785	-1.834

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.276 + 2.692 \times 10^{-3}T - 1.341 \times 10^{5}T^{-2}$

$H° - H°_{298} = 9.276 \times 10^{-3}T + 1.346 \times 10^{-6}T^{2} + 1.341 \times 10^{2}T^{-1} - 3.335$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 32.598 - 0.729 \times 10^{-3}T + 0.076 \times 10^{-6}T^{2} - 26.000T^{-1}$

$\Delta Gf° = 32.598 + 0.729 \times 10^{-3}T\ln T - 0.076 \times 10^{-6}T^{2} - 13.000T^{-1} - 13.332 \times 10^{-3}T$

Source: Data from JANAF (127).

HCNO(g)
Hydrogen Isocyanate (ideal gas)
[Formation: $0.5H_2(g) + C(c) + 0.5N_2(g) + 0.5O_2(g) = HCNO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	10.765	56.911	56.911	0	-24.300	-22.078	16.184
300	10.793	56.978	56.911	.020	-24.303	-22.065	16.074
400	12.124	60.274	57.351	1.169	-24.449	-21.294	11.635
500	13.147	63.094	58.224	2.435	-24.566	-20.492	8.957
600	13.960	65.565	59.247	3.791	-24.671	-19.667	7.164
700	14.634	67.769	60.309	5.222	-24.768	-18.825	5.877
800	15.207	69.762	61.368	6.715	-24.858	-17.970	4.909
900	15.703	71.582	62.403	8.261	-24.941	-17.105	4.154
1000	16.136	73.260	63.407	9.853	-25.016	-16.232	3.547
1100	16.516	74.816	64.374	11.486	-25.083	-15.339	3.047
1200	16.849	76.268	65.305	13.155	-25.144	-14.460	2.634
1300	17.142	77.628	66.201	14.855	-25.201	-13.567	2.281
1400	17.400	78.908	67.064	16.582	-25.253	-12.671	1.978
1500	17.627	80.116	67.893	18.334	-25.302	-11.770	1.715
1600	17.827	81.261	68.694	20.107	-25.348	-10.867	1.484
1700	18.005	82.347	69.466	21.898	-25.395	-9.962	1.281
1800	18.162	83.380	70.209	23.707	-25.440	-9.050	1.099
1900	18.302	84.366	70.929	25.530	-25.485	-8.139	.936
2000	18.426	85.308	71.624	27.367	-25.532	-7.224	.789

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.730 + 3.382 \times 10^{-3}T - 2.643 \times 10^{5}T^{-2}$

$H° - H°_{298} = 12.730 \times 10^{-3}T + 1.691 \times 10^{-6}T^{2} + 2.643 \times 10^{2}T^{-1} - 4.832$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -24.324 - 0.890 \times 10^{-3}T + 0.169 \times 10^{-6}T^{2} + 81.600T^{-1}$

$\Delta Gf° = -24.324 + 0.890 \times 10^{-3}T\ln T - 0.169 \times 10^{-6}T^{2} + 40.800T^{-1} + 2.055 \times 10^{-3}T$

Source: Data from Chase (81).

$HNO_3(g)$
Nitric Acid (ideal gas)
[Formation: $0.5H_2(g) + 0.5N_2(g) + 1.5O_2(g) = HNO_3(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	12.748	63.663	63.663	0	-32.100	-17.690	12.967
300	12.795	63.742	63.663	.024	-32.109	-17.600	12.821
400	15.103	67.750	64.192	1.423	-32.470	-12.703	6.941
500	16.930	71.325	65.269	3.028	-32.662	-7.736	3.381
600	18.348	74.543	66.551	4.795	-32.734	-2.743	.999
700	19.451	77.458	67.905	6.687	-32.724	2.256	-.704
800	20.325	80.114	69.267	8.678	-32.654	7.248	-1.980
900	21.031	82.550	70.609	10.747	-32.542	12.230	-2.970
1000	21.613	84.797	71.917	12.880	-32.396	17.196	-3.758
1100	22.098	86.880	73.184	15.066	-32.225	22.149	-4.400
1200	22.508	88.821	74.407	17.297	-32.034	27.084	-4.933
1300	22.858	90.637	75.586	19.566	-31.827	32.002	-5.380
1400	23.159	92.342	76.723	21.867	-31.611	36.904	-5.761
1500	23.419	93.949	77.818	24.196	-31.385	41.789	-6.089
1600	23.646	95.468	78.874	26.550	-31.153	46.659	-6.373
1700	23.843	96.908	79.894	28.924	-30.917	51.515	-6.623
1800	24.017	98.276	80.878	31.317	-30.679	56.358	-6.843
1900	24.170	99.578	81.827	33.727	-30.439	61.188	-7.038
2000	24.306	100.822	82.746	36.151	-30.200	66.002	-7.212

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 17.281 + 4.324\times10^{-3}T - 5.176\times10^{5}T^{-2}$

$H° - H°_{298} = 17.281\times10^{-3}T + 2.162\times10^{-6}T^{2} + 5.176\times10^{2}T^{-1} - 7.081$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -33.715 - 0.051\times10^{-3}T + 0.903\times10^{-6}T^{2} + 462.000T^{-1}$

$\Delta Gf° = -33.715 + 0.051\times10^{-3}T\ln T - 0.903\times10^{-6}T^{2} + 231.000T^{-1} + 51.132\times10^{-3}T$

Source: Data from JANAF (127).

$HOCl(g)$
Hydrogen Oxychloride (ideal gas)
[Formation: $0.5H_2(g) + 0.5O_2(g) + 0.5Cl_2(g) = HOCl(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.911	56.521	56.521	0	-17.800	-14.750	10.812
300	8.924	56.576	56.523	.016	-17.804	-14.731	10.732
400	9.579	59.235	56.880	.942	-17.996	-13.677	7.473
500	10.112	61.432	57.576	1.928	-18.151	-12.578	5.498
600	10.527	63.314	58.379	2.961	-18.280	-11.451	4.171
700	10.860	64.963	59.204	4.031	-18.389	-10.304	3.217
800	11.139	66.431	60.017	5.131	-18.484	-9.143	2.498
900	11.383	67.758	60.806	6.257	-18.566	-7.971	1.936
1000	11.601	68.968	61.561	7.407	-18.635	-6.789	1.484
1100	11.799	70.084	62.287	8.577	-18.696	-5.602	1.113
1200	11.978	71.118	62.980	9.766	-18.749	-4.408	.803
1300	12.142	72.083	63.643	10.972	-18.795	-3.211	.540
1400	12.289	72.989	64.279	12.194	-18.835	-2.012	.314
1500	12.423	73.841	64.888	13.429	-18.872	-.809	.118
1600	12.543	74.647	65.473	14.678	-18.903	.396	-.054
1700	12.652	75.411	66.036	15.938	-18.933	1.604	-.206
1800	12.750	76.137	66.577	17.208	-18.960	2.812	-.341
1900	12.838	76.828	67.098	18.487	-18.988	4.024	-.463
2000	12.918	77.489	67.602	19.775	-19.014	5.235	-.572

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.830 + 1.780\times10^{-3}T - 1.289\times10^{5}T^{-2}$
$H°-H°_{298} = 9.830\times10^{-3}T + 0.890\times10^{-6}T^{2} + 1.289\times10^{2}T^{-1} - 3.442$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -17.679 - 1.427\times10^{-3}T + 0.385\times10^{-6}T^{2} + 80.400T^{-1}$
$\Delta Gf° = -17.679 + 1.427\times10^{-3}T\ln T - 0.385\times10^{-6}T^{2} + 40.200T^{-1} + 1.358\times10^{-3}T$

Source: Data from JANAF (129).

$HOF(g)$
Hydrogen Oxyfluoride (ideal gas)
[Formation: $0.5H_2(g) + 0.5O_2(g) + 0.5F_2(g) = HOF(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	8.589	54.169	54.169	0	-23.160	-20.131	14.756
300	8.600	54.223	54.173	.015	-23.165	-20.114	14.653
400	9.219	56.782	54.515	.907	-23.360	-19.065	10.416
500	9.777	58.901	55.185	1.858	-23.525	-17.971	7.855
600	10.237	60.726	55.961	2.859	-23.667	-16.847	6.137
700	10.617	62.333	56.759	3.902	-23.788	-15.701	4.902
800	10.938	63.773	57.547	4.981	-23.892	-14.539	3.972
900	11.218	65.077	58.313	6.088	-23.983	-13.364	3.245
1000	11.467	66.273	59.050	7.223	-24.061	-12.181	2.662
1100	11.689	67.376	59.757	8.381	-24.128	-10.989	2.183
1200	11.888	68.402	60.435	9.560	-24.187	-9.791	1.783
1300	12.067	69.361	61.085	10.759	-24.236	-8.589	1.444
1400	12.228	70.261	61.709	11.973	-24.282	-7.385	1.153
1500	12.371	71.110	62.308	13.203	-24.322	-6.177	.900
1600	12.500	71.912	62.883	14.446	-24.359	-4.966	.678
1700	12.616	72.674	63.436	15.704	-24.389	-3.751	.482
1800	12.719	73.398	63.970	16.971	-24.421	-2.536	.308
1900	12.812	74.088	64.484	18.247	-24.451	-1.319	.152
2000	12.895	74.747	64.982	19.530	-24.484	-.103	.011

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.265 + 2.148\times10^{-3}T - 1.170\times10^{5}T^{-2}$
$H°- H°_{298} = 9.265\times10^{-3}T + 1.074\times10^{-6}T^{2} + 1.170\times10^{2}T^{-1} - 3.250$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -22.836 - 1.832\times10^{-3}T + 0.526\times10^{-6}T^{2} + 52.400T^{-1}$
$\Delta Gf° = -22.836 + 1.832\times10^{-3}T\ln T - 0.526\times10^{-6}T^{2} + 26.200T^{-1} - 1.503\times10^{-3}T$

Source: Data from Gurvich (194).

HOI(g)
Hydrogen Oxyiodide (ideal gas)
[Formation: $0.5H_2(g) + 0.5O_2(g) + 0.5I_2(c,l,g) = HOI(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	9.312	60.868	60.868	0	-88.550	-90.602	66.412
300	9.326	60.925	60.868	.017	-88.558	-90.615	66.012
386.8	9.886	63.367	61.167	.851	-88.937	-91.162	51.508
386.8	9.886	63.367	61.167	.851	-90.791	-91.162	51.508
400	9.971	63.700	61.245	.982	-90.881	-91.173	49.814
458.4	10.255	65.080	61.646	1.574	-91.267	-91.187	43.474
458.4	10.255	65.080	61.646	1.574	-96.278	-91.187	43.474
500	10.457	65.980	61.970	2.005	-96.332	-90.722	39.654
600	10.820	67.921	62.803	3.071	-96.442	-89.589	32.632
700	11.104	69.610	63.656	4.168	-96.535	-88.438	27.611
800	11.343	71.109	64.498	5.289	-96.616	-87.278	23.843
900	11.556	72.457	65.308	6.434	-96.686	-86.106	20.909
1000	11.750	73.685	66.085	7.600	-96.745	-84.927	18.561
1100	11.926	74.814	66.829	8.783	-96.798	-83.744	16.638
1200	12.089	75.858	67.536	9.986	-96.841	-82.552	15.035
1300	12.240	76.833	68.216	11.202	-96.881	-81.362	13.678
1400	12.376	77.744	68.863	12.433	-96.916	-80.165	12.514
1500	12.500	78.602	69.485	13.676	-96.948	-78.969	11.506
1600	12.612	79.412	70.080	14.931	-96.977	-77.769	10.623
1700	12.713	80.179	70.651	16.197	-97.003	-76.566	9.843
1800	12.806	80.908	71.200	17.474	-97.027	-75.362	9.150
1900	12.890	81.604	71.730	18.760	-97.051	-74.159	8.530
2000	12.964	82.266	72.241	20.050	-97.078	-72.954	7.972

*Enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.229 + 1.558\times10^{-3}T - 1.228\times10^{5}T^{-2}$

$H°-H°_{298} = 10.229\times10^{-3}T + 0.779\times10^{-6}T^{2} + 1.228\times10^{2}T^{-1} - 3.531$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -87.966 - 3.053\times10^{-3}T - 0.428\times10^{-6}T^{2} + 108.450T^{-1}$

$\Delta Gf° = -87.966 + 3.053\times10^{-3}T\ln T + 0.428\times10^{-6}T^{2} + 54.225T^{-1} - 26.973\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -88.693 - 6.255\times10^{-3}T + 0.318\times10^{-6}T^{2} + 108.450T^{-1}$

$\Delta Gf° = -88.693 + 6.255\times10^{-3}T\ln T - 0.318\times10^{-6}T^{2} + 54.225T^{-1} - 43.880\times10^{-3}T$

458.4-2000 K: $\Delta Hf° = -96.050 - 1.085\times10^{-3}T + 0.284\times10^{-6}T^{2} + 100.800T^{-1}$

$\Delta Gf° = -96.050 + 1.085\times10^{-3}T\ln T - 0.284\times10^{-6}T^{2} + 50.400T^{-1} + 3.851\times10^{-3}T$

Source: Data from Garisto (171) who estimated Gibbs energy of formation at 298 K.

$H_3PO_4(c,l)$
Orthophosphoric Acid
[Formation: $1.5H_2(g) + P(c,l,1/4P_4(g)) + 2O_2(g) = H_3PO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	25.350	26.421	26.421	0	-305.700	-267.471	196.059
300	25.480	26.578	26.421	.047	-305.710	-267.235	194.678
315.5*	26.610	27.860	26.434	.450	-305.774	-265.235	183.729
315.5	35.920	38.003	26.434	3.650	-302.574	-265.235	183.729
317.3	36.050	38.208	26.500	3.715	-302.563	-265.022	182.540
317.3	36.050	38.208	26.500	3.715	-302.720	-265.022	182.540
400	42.000	47.248	29.893	6.942	-302.052	-255.278	139.476
500	49.200	57.394	34.390	11.502	-300.631	-243.735	106.535
550	52.800	62.249	36.700	14.052	-299.670	-238.104	94.612
550	52.800	62.249	36.700	14.052	-302.578	-238.104	94.612
600	56.400	67.000	39.030	16.782	-301.367	-232.295	84.612
700	63.600	76.235	43.689	22.782	-298.448	-221.004	69.000
800	70.800	85.198	48.320	29.502	-294.861	-210.180	57.418
900	78.000	93.953	52.906	36.942	-290.598	-199.843	48.528
1000	85.200	102.543	57.441	45.102	-285.654	-190.019	41.528

*Data above 300 K estimated except temperature and enthalpy of fusion.

Phase changes: 315.5 K, melting point of H_3PO_4; $\Delta H° = 3.200$ kcal/mol.
317.3 K, melting point of P; $\Delta H° = 0.157$ kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H° = 2.908$ kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-315.5 K: $Cp° = 3.699 + 72.600\times10^{-3}T$
$H°- H°_{298} = 3.699\times10^{-3}T + 36.300\times10^{-6}T^2 - 4.330$
315.5-1000 K: $Cp° = 13.200 + 72.000\times10^{-3}T$
$H°- H°_{298} = 13.200\times10^{-3}T + 36.000\times10^{-6}T^2 - 4.098$

Formation equations (kcal/mol):

298.15-315.5 K: $\Delta Hf° = -301.050 - 24.244\times10^{-3}T + 31.480\times10^{-6}T^2 - 65.650T^{-1}$
$\Delta Gf° = -301.050 + 24.244\times10^{-3}T\ln T - 31.480\times10^{-6}T^2 - 32.825T^{-1} - 15.755\times10^{-3}T$
315.5-317.3 K: $\Delta Hf° = -300.818 - 14.743\times10^{-3}T + 31.180\times10^{-6}T^2 - 65.650T^{-1}$
$\Delta Gf° = -300.818 + 14.743\times10^{-3}T\ln T - 31.180\times10^{-6}T^2 - 32.825T^{-1} + 38.085\times10^{-3}T$
317.3-550 K: $\Delta Hf° = -300.504 - 17.236\times10^{-3}T + 34.365\times10^{-6}T^2 - 65.650T^{-1}$
$\Delta Gf° = -300.504 + 17.236\times10^{-3}T\ln T - 34.365\times10^{-6}T^2 - 32.825T^{-1} + 23.749\times10^{-3}T$
550-1000 K: $\Delta Hf° = -303.965 - 15.898\times10^{-3}T + 34.361\times10^{-6}T^2 - 165.950T^{-1}$
$\Delta Gf° = -303.965 + 15.898\times10^{-3}T\ln T - 34.361\times10^{-6}T^2 - 82.975T^{-1} + 38.646\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data from Chase (81) who estimated all except temperature and enthalpy of fusion.

$H_2Se(g)$
Dihydrogen Selenide (ideal gas)
[Reaction: $H_2(g) + 0.5Se(g) = H_2Se(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hr°$	$\Delta Gr°$	
298.15	8.280	52.300	52.300	0	-21.125	-21.121	15.482
300	8.300	52.350	52.300	.016	-21.127	-21.120	15.386
400	8.800	54.810	52.630	.872	-21.219	-21.104	11.530
500	9.220	56.820	53.274	1.773	-21.276	-21.068	9.208
600	9.600	58.540	54.017	2.714	-21.297	-21.026	7.659
700	9.980	60.050	54.774	3.693	-21.286	-20.986	6.552
800	10.340	61.400	55.514	4.709	-21.244	-20.938	5.720
900	10.700	62.640	56.239	5.761	-21.173	-20.904	5.076
1000	11.060	63.790	56.941	6.849	-21.076	-20.885	4.564
1100	11.410	64.860	57.612	7.973	-20.952	-20.873	4.147
1200	11.770	65.870	58.260	9.132	-20.805	-20.873	3.802
1300	12.120	66.820	58.876	10.327	-20.634	-20.875	3.509
1400	12.470	67.730	59.476	11.556	-20.442	-20.897	3.262
1500	12.830	68.610	60.063	12.821	-20.226	-20.955	3.053
1600	13.180	69.440	60.614	14.122	-19.986	-20.993	2.868
1700	13.530	70.250	61.158	15.457	-19.723	-21.061	2.708
1800	13.880	71.040	61.692	16.827	-19.438	-21.161	2.569
1900	14.230	71.800	62.204	18.233	-19.128	-21.267	2.446
2000	14.580	72.540	62.703	19.674	-18.793	-21.389	2.337

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.596 + 3.496\times10^{-3}T - 0.319\times10^{5}T^{-2}$

$H°-H°_{298} = 7.596\times10^{-3}T + 1.748\times10^{-6}T^{2} + 0.319\times10^{2}T^{-1} - 2.527$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -20.935 - 1.426\times10^{-3}T + 1.240\times10^{-6}T^{2} + 37.350T^{-1}$

$\Delta Gr° = -20.935 + 1.426\times10^{-3}T\ln T - 1.240\times10^{-6}T^{2} + 18.675T^{-1} - 8.590\times10^{-3}T$

Source: Data from Mills (332).

$H_2Te(g)$
Dihydrogen Telluride (ideal gas)
[Reaction: $H_2(g) + 0.5Te(g) = H_2Te(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	8.500	54.700	54.700	0	-1.500	-1.999	1.465
300	8.520	54.750	54.700	.016	-1.501	-2.001	1.458
400	9.170	57.300	55.040	.904	-1.555	-2.156	1.178
500	9.620	59.400	55.712	1.844	-1.561	-2.308	1.009
600	10.000	61.190	56.480	2.826	-1.526	-2.460	.896
700	10.340	62.760	57.269	3.844	-1.458	-2.624	.819
800	10.670	64.160	58.043	4.894	-1.364	-2.794	.763
900	10.980	65.440	58.799	5.977	-1.244	-2.986	.725
1000	11.290	66.610	59.520	7.090	-1.103	-3.183	.696
1100	11.590	67.700	60.215	8.234	-.940	-3.397	.675
1200	11.880	68.720	60.880	9.408	-.760	-3.625	.660
1300	12.180	69.680	61.518	10.611	-.564	-3.872	.651
1400	12.470	70.600	62.140	11.844	-.349	-4.143	.647
1500	12.770	71.470	62.733	13.106	-.119	-4.417	.644
1600	13.060	72.300	63.302	14.397	.129	-4.711	.643
1700	13.350	73.100	63.855	15.717	.393	-5.024	.646
1800	13.640	73.870	64.388	17.067	.676	-5.349	.649
1900	13.930	74.620	64.912	18.446	.976	-5.695	.655
2000	14.220	75.340	65.413	19.853	1.292	-6.053	.661

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.489 + 2.874 \times 10^{-3}T - 0.752 \times 10^{5}T^{-2}$

$H° - H°_{298} = 8.489 \times 10^{-3}T + 1.437 \times 10^{-6}T^{2} + 0.752 \times 10^{2}T^{-1} - 2.911$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -1.831 - 0.290 \times 10^{-3}T + 0.910 \times 10^{-6}T^{2} + 100.300T^{-1}$

$\Delta Gr° = -1.831 + 0.290 \times 10^{-3}T\ln T - 0.910 \times 10^{-6}T^{2} + 50.150T^{-1} - 2.512 \times 10^{-3}T$

Source: Data from Mills (332).

$HfB_2(c)$
Hafnium Diboride
[Formation: $Hf(c) + 2B(\beta) = HfB_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.890	10.200	10.200	0	-80.300	-79.397	58.199
300	11.962	10.274	10.201	.022	-80.299	-79.388	57.834
400	14.661	14.139	10.709	1.372	-80.208	-79.104	43.220
500	16.107	17.579	11.747	2.916	-80.120	-78.830	34.456
600	17.079	20.606	12.976	4.578	-80.069	-78.585	28.624
700	17.827	23.297	14.263	6.324	-80.038	-78.335	24.457
800	18.455	25.719	15.545	8.139	-80.013	-78.092	21.334
900	19.015	27.926	16.800	10.013	-79.992	-77.855	18.906
1000	19.531	29.956	18.015	11.941	-79.974	-77.620	16.964
1100	20.019	31.841	19.187	13.919	-79.956	-77.394	15.377
1200*	20.488	33.603	20.316	15.944	-79.939	-77.159	14.052
1300	20.943	35.261	21.403	18.016	-79.924	-76.922	12.932
1400	21.389	36.829	22.449	20.132	-79.910	-76.689	11.971
1500	21.827	38.320	23.458	22.293	-79.900	-76.450	11.139

*Data above 1150 K extrapolated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 15.912 + 4.080\times10^{-3}T - 4.610\times10^{5}T^{-2}$

$H°-H°_{298} = 15.912\times10^{-3}T + 2.040\times10^{-6}T^{2} + 4.610\times10^{2}T^{-1} - 6.472$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = -80.593 + 0.857\times10^{-3}T - 0.254\times10^{-6}T^{2} + 18.000T^{-1}$

$\Delta Gf° = -80.593 - 0.857\times10^{-3}T\ln T + 0.254\times10^{-6}T^{2} + 9.000T^{-1} + 8.720\times10^{-3}T$

Sources: Data at 298 K from Wagman (515). Other data based on Mezaki (331). Data above 1150 K extrapolated.

$HfC(c)$
Hafnium Carbide
[Formation: $Hf(c,l) + C(c) = HfC(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.960	9.474	9.474	0	-54.000	-53.312	39.078
300	9.000	9.529	9.474	.020	-53.995	-53.303	38.831
400	10.250	12.309	9.859	.980	-53.904	-53.098	29.011
500	10.880	14.680	10.620	2.030	-53.813	-52.919	23.131
600	11.290	16.709	11.476	3.140	-53.741	-52.754	19.215
700	11.610	18.480	12.351	4.290	-53.694	-52.591	16.419
800	11.860	20.050	13.225	5.460	-53.681	-52.442	14.326
900	12.070	21.460	14.060	6.660	-53.683	-52.287	12.697
1000	12.250	22.739	14.869	7.870	-53.714	-52.138	11.395
1100	12.420	23.925	15.643	9.110	-53.750	-51.969	10.325
1200	12.560	25.000	16.367	10.360	-53.808	-51.800	9.434
1300	12.700	26.028	17.090	11.620	-53.887	-51.658	8.684
1400	12.840	26.984	17.770	12.900	-53.972	-51.490	8.038
1500	12.980	27.868	18.408	14.190	-54.075	-51.299	7.474
1600	13.120	28.705	19.024	15.490	-54.192	-51.112	6.981
1700	13.250	29.517	19.629	16.810	-54.316	-50.942	6.549
1800	13.380	30.258	20.180	18.140	-54.452	-50.690	6.155
1900	13.520	30.999	20.741	19.490	-54.592	-50.509	5.810
2000	13.660	31.692	21.267	20.850	-54.746	-50.280	5.494
2013	13.672	31.781	21.335	21.028	-54.766	-50.251	5.456
2013	13.672	31.781	21.335	21.028	-56.376	-50.251	5.456
2100	13.750	32.361	21.780	22.220	-56.398	-49.989	5.202
2200	13.940	33.031	22.299	23.610	-56.420	-49.734	4.941
2300	14.080	33.652	22.778	25.010	-56.455	-49.424	4.696
2400	14.220	34.250	23.242	26.420	-56.513	-49.114	4.472
2470	14.318	34.674	23.577	27.410	-56.570	-48.940	4.330
2470	14.318	34.674	23.577	27.410	-62.250	-48.940	4.330
2500	14.360	34.847	23.711	27.840	-62.246	-48.778	4.264
2600	14.520	35.421	24.148	29.310	-62.198	-48.233	4.054
2700	14.670	35.970	24.566	30.790	-62.143	-47.671	3.859
2800	14.820	36.496	24.989	32.220	-62.141	-47.153	3.680
2900	14.970	37.022	25.398	33.710	-62.082	-46.625	3.514
3000	15.130	37.548	25.808	35.220	-62.007	-46.137	3.361

Phase changes: 2013 K, α - β transition point of Hf; ΔH° = 1.610 kcal/mol.
2470 K, melting point of Hf; ΔH° = 5.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 11.171 + 1.280\times10^{-3}T - 2.305\times10^{5}T^{-2}$
$H°-H°_{298} = 11.171\times10^{-3}T + 0.640\times10^{-6}T^{2} + 2.305\times10^{2}T^{-1} - 4.161$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -54.713 + 2.044\times10^{-3}T - 1.036\times10^{-6}T^{2} + 58.200T^{-1}$
$\Delta Gf° = -54.713 - 2.044\times10^{-3}T\ln T + 1.036\times10^{-6}T^{2} + 29.100T^{-1} + 15.707\times10^{-3}T$
2000-2013 K: $\Delta Hf° = -52.721 - 0.079\times10^{-3}T - 0.404\times10^{-6}T^{2} - 489.500T^{-1}$
$\Delta Gf° = -52.721 + 0.079\times10^{-3}T\ln T + 0.404\times10^{-6}T^{2} - 244.750T^{-1} - 0.093\times10^{-3}T$
2013-2470 K: $\Delta Hf° = -58.010 + 2.101\times10^{-3}T - 0.579\times10^{-6}T^{2} - 489.500T^{-1}$
$\Delta Gf° = -58.010 - 2.101\times10^{-3}T\ln T + 0.579\times10^{-6}T^{2} - 244.750T^{-1} + 18.767\times10^{-3}T$
2470-3000 K: $\Delta Hf° = -59.019 - 2.470\times10^{-3}T + 0.506\times10^{-6}T^{2} - 489.500T^{-1}$
$\Delta Gf° = -59.019 + 2.470\times10^{-3}T\ln T - 0.506\times10^{-6}T^{2} - 244.750T^{-1} - 13.853\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Spencer (472). Other data from Turchanin (507).

HfN(c)
Hafnium Nitride
[Formation: $Hf(c) + 0.5N_2(g) = HfN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	9.420	11.500	11.500	0	-89.300	-82.802	60.695
300	9.450	11.558	11.500	.020	-89.298	-82.758	60.288
400	10.380	14.419	11.894	1.010	-89.281	-80.589	44.031
500	10.930	16.798	12.638	2.080	-89.204	-78.417	34.276
600	11.320	18.827	13.494	3.200	-89.102	-76.265	27.779
700	11.650	20.597	14.397	4.340	-89.005	-74.139	23.147
800	11.930	22.172	15.272	5.520	-88.894	-72.024	19.676
900	12.200	23.592	16.114	6.730	-88.779	-69.920	16.979
1000	12.450	24.890	16.930	7.960	-88.670	-67.836	14.825
1100	12.690	26.088	17.706	9.220	-88.556	-65.751	13.063
1200	12.920	27.202	18.452	10.500	-88.446	-63.683	11.598
1300	13.150	28.245	19.168	11.800	-88.340	-61.629	10.361
1400	13.380	29.228	19.849	13.130	-88.227	-59.571	9.299
1500	13.600	30.159	20.506	14.480	-88.117	-57.526	8.381
1600	13.820	31.044	21.138	15.850	-88.008	-55.499	7.581
1700	14.050	31.889	21.748	17.240	-87.901	-53.479	6.875
1800	14.270	32.698	22.331	18.660	-87.784	-51.438	6.245
1900	14.490	33.475	22.896	20.100	-87.669	-49.430	5.686
2000	14.700	34.224	23.444	21.560	-87.554	-47.421	5.182
2013	14.729	34.319	23.514	21.751	-87.538	-47.159	5.120
2013	14.729	34.319	23.514	21.751	-89.148	-47.159	5.120
2100	14.920	34.946	23.975	23.040	-88.924	-45.351	4.720
2200	15.140	35.646	24.491	24.540	-88.663	-43.286	4.300

*Entropy at 298 K estimated.

Phase change: 2013 K, α - β transition point of Hf; ΔH° = 1.610 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2200 K: $Cp° = 10.446 + 2.148\times10^{-3}T - 1.480\times10^{5}T^{-2}$

$H°- H°_{298} = 10.446\times10^{-3}T + 1.074\times10^{-6}T^{2} + 1.480\times10^{2}T^{-1} - 3.706$

Formation equations (kcal/mol):

298.15-2000 K: $ΔHf° = -90.269 + 1.578\times10^{-3}T - 0.130\times10^{-6}T^{2} + 151.950T^{-1}$

$ΔGf° = -90.269 - 1.578\times10^{-3}T\ln T + 0.130\times10^{-6}T^{2} + 75.975T^{-1} + 33.144\times10^{-3}T$

2000-2013 K: $ΔHf° = -88.932 + 0.514\times10^{-3}T + 0.136\times10^{-6}T^{2} - 398.000T^{-1}$

$ΔGf° = -88.932 - 0.514\times10^{-3}T\ln T - 0.136\times10^{-6}T^{2} - 199.000T^{-1} + 24.990\times10^{-3}T$

2013-2200 K: $ΔHf° = -94.221 + 2.694\times10^{-3}T - 0.039\times10^{-6}T^{2} - 398.000T^{-1}$

$ΔGf° = -94.221 - 2.694\times10^{-3}T\ln T + 0.039\times10^{-6}T^{2} - 199.000T^{-1} + 43.849\times10^{-3}T$

Sources: Enthalpy of formation and estimated entropy at 298 K from Spencer (472). Other data from Litvinenko (310).

$HfO(g)$
Hafnium Monoxide (ideal gas)
[Formation: $Hf(c,l) + 0.5O_2(g) = HfO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.430	56.285	56.285	0	16.000	9.628	-7.057
300	7.430	56.332	56.285	.014	15.997	9.589	-6.986
400	7.740	58.504	56.579	.770	15.773	7.485	-4.090
500	8.040	60.268	57.146	1.561	15.556	5.442	-2.379
600	8.260	61.756	57.794	2.377	15.334	3.437	-1.252
700	8.420	63.040	58.453	3.211	15.100	1.476	-.461
800	8.530	64.172	59.099	4.058	14.850	-.456	.125
900	8.610	65.182	59.720	4.916	14.586	-2.355	.572
1000	8.680	66.093	60.312	5.781	14.303	-4.225	.923
1100	8.730	66.922	60.876	6.651	14.002	-6.059	1.204
1200	8.770	67.684	61.412	7.526	13.683	-7.869	1.433
1300	8.800	68.387	61.922	8.405	13.345	-9.653	1.623
1400	8.830	69.041	62.408	9.286	12.988	-11.407	1.781
1500	8.850	69.651	62.870	10.171	12.612	-13.134	1.914
1600	8.870	70.223	63.312	11.057	12.217	-14.845	2.028
1700	8.890	70.761	63.735	11.945	11.802	-16.527	2.125
1800	8.900	71.271	64.140	12.835	11.369	-18.169	2.206
1900	8.920	71.752	64.528	13.726	10.915	-19.807	2.278
2000	8.930	72.209	64.900	14.618	10.441	-21.410	2.340
2013	8.931	72.267	64.947	14.734	10.379	-21.617	2.347
2013	8.931	72.267	64.947	14.734	8.769	-21.617	2.347
2100	8.940	72.645	65.259	15.511	8.462	-22.925	2.386
2200	8.950	73.061	65.604	16.406	8.096	-24.410	2.425
2300	8.960	73.460	65.937	17.302	7.709	-25.880	2.459
2400	8.970	73.842	66.260	18.198	7.292	-27.333	2.489
2470	8.977	74.099	66.477	18.826	6.979	-28.336	2.507
2470	8.977	74.099	66.477	18.826	1.299	-28.336	2.507
2500	8.980	74.207	66.569	19.095	1.189	-28.695	2.509

Phase changes: 2013 K, α - β transition point of Hf; ΔH° = 1.610 kcal/mol.
2470 K, melting point of Hf; ΔH° = 5.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 8.323 + 0.346\times10^{-3}T - 0.885\times10^{5}T^{-2}$
$H°-H°_{298} = 8.323\times10^{-3}T + 0.173\times10^{-6}T^2 + 0.885\times10^{2}T^{-1} - 2.794$

Formation equations (kcal/mol):

298.15-2000 K: $ΔHf° = 16.135 - 0.901\times10^{-3}T - 0.988\times10^{-6}T^2 + 65.900T^{-1}$
$ΔGf° = 16.135 + 0.901\times10^{-3}T\ln T + 0.988\times10^{-6}T^2 + 32.950T^{-1} - 27.626\times10^{-3}T$
2000-2013 K: $ΔHf° = 16.804 - 1.456\times10^{-3}T - 0.841\times10^{-6}T^2 - 226.500T^{-1}$
$ΔGf° = 16.804 + 1.456\times10^{-3}T\ln T + 0.841\times10^{-6}T^2 - 113.250T^{-1} - 31.848\times10^{-3}T$
2013-2470 K: $ΔHf° = 11.514 + 0.724\times10^{-3}T - 1.016\times10^{-6}T^2 - 226.500T^{-1}$
$ΔGf° = 11.514 - 0.724\times10^{-3}T\ln T + 1.016\times10^{-6}T^2 - 113.250T^{-1} - 12.989\times10^{-3}T$
2470-2500 K: $ΔHf° = 10.505 - 3.847\times10^{-3}T + 0.068\times10^{-6}T^2 - 226.500T^{-1}$
$ΔGf° = 10.505 + 3.847\times10^{-3}T\ln T - 0.068\times10^{-6}T^2 - 113.250T^{-1} - 45.609\times10^{-3}T$

Source: Data from Pedley (396).

HgSe(c)
Mercury Selenide
[Reaction: $Hg(l,g) + 0.5Se_2(g) = HgSe(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	12.800	24.100	24.100	0	-29.750	-22.851	16.750
300	12.810	24.180	24.100	.024	-29.747	-22.808	16.615
400	13.180	27.920	24.608	1.325	-29.605	-20.515	11.209
500	13.550	30.900	25.578	2.661	-29.425	-18.263	7.982
600*	13.920	33.410	26.685	4.035	-29.205	-16.055	5.848
629.81	14.030	34.088	27.019	4.452	-29.132	-15.402	5.345
629.81	14.030	34.088	27.019	4.452	-43.283	-15.402	5.345
700	14.290	35.580	27.801	5.445	-42.992	-12.306	3.842
800	14.660	37.510	28.894	6.893	-42.545	-7.949	2.172
900	15.030	39.260	29.952	8.377	-42.060	-3.656	.888
1000	15.400	40.860	30.961	9.899	-41.535	.585	-.128

*Data extrapolated above 510 K.

Phase change: 629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 11.700 + 3.700\times10^{-3}T$
$H°-H°_{298} = 11.700\times10^{-3}T + 1.850\times10^{-6}T^2 - 3.653$

Reaction equations (kcal/mol):

298.15-629.81 K: $\Delta Hr° = -29.953 + 0.095\times10^{-3}T + 1.909\times10^{-6}T^2 + 1.450T^{-1}$
$\Delta Gr° = -29.953 - 0.095\times10^{-3}T\ln T - 1.909\times10^{-6}T^2 + 0.725T^{-1} + 24.922\times10^{-3}T$
629.81-1000 K: $\Delta Hr° = -44.916 + 1.400\times10^{-3}T + 2.009\times10^{-6}T^2 - 29.950T^{-1}$
$\Delta Gr° = -44.916 - 1.400\times10^{-3}T\ln T - 2.009\times10^{-6}T^2 - 14.975T^{-1} + 57.195\times10^{-3}T$

Source: Enthalpy of formation at 298 K from Imperatori (213). Other data from Mills (332) who extrapolated above 510 K.

HgTe(c)
Mercury Telluride
[Reaction: $Hg(l,g) + 0.5Te_2(g) = HgTe(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	13.100	27.000	27.000	0	-25.965	-19.383	14.208
300*	13.100	27.080	27.000	.025	-25.960	-19.342	14.090
400	13.320	30.880	27.515	1.346	-25.740	-17.168	9.380
500	13.540	33.880	28.504	2.688	-25.498	-15.056	6.581
600	13.750	36.360	29.605	4.053	-25.238	-12.985	4.730
629.81	13.816	37.028	29.941	4.464	-25.158	-12.377	4.295
629.81	13.816	37.028	29.941	4.464	-39.309	-12.377	4.295
700	13.970	38.500	30.730	5.439	-39.009	-9.394	2.933
800	14.190	40.380	31.823	6.846	-38.571	-5.196	1.419
900	14.400	42.060	32.864	8.276	-38.119	-1.047	.254
943	14.500	42.730	33.295	8.897	-37.921	.723	-.168

*Data above 298 K except temperature of fusion estimated.

Phase changes: 629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol
943 K, melting point of HgTe; ΔH° = 8.7±1.3 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-943 K: $Cp° = 12.450 + 2.170\times10^{-3}T$
$H° - H^\circ_{298} = 12.450\times10^{-3}T + 1.085\times10^{-6}T^2 - 3.808$

Reaction equations (kcal/mol):

298.15-629.81 K: $\Delta Hr° = -26.651 + 1.878\times10^{-3}T + 0.687\times10^{-6}T^2 + 19.300T^{-1}$
$\Delta Gr° = -26.651 - 1.878\times10^{-3}T\ln T - 0.687\times10^{-6}T^2 + 9.650T^{-1} + 35.168\times10^{-3}T$
629.81-943 K: $\Delta Hr° = -41.614 + 3.182\times10^{-3}T + 0.789\times10^{-6}T^2 - 12.100T^{-1}$
$\Delta Gr° = -41.614 - 3.182\times10^{-3}T\ln T - 0.789\times10^{-6}T^2 - 6.050T^{-1} + 67.441\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Su (485). Other data from Mills (332) who estimated all above 298 K except temperature of fusion. Enthalpy of fusion from Su (485).

HoN(c)
Holmium Nitride
[Formation: Ho(c,l) + $0.5N_2(g)$ = HoN(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.800	19.000	19.000	0	-80.500	-73.996	54.240
300	11.810	19.070	19.003	.020	-80.499	-73.957	53.877
400	11.940	22.490	19.465	1.210	-80.315	-71.803	39.231
500	12.080	25.170	20.350	2.410	-80.136	-69.695	30.463
600	12.210	27.380	21.347	3.620	-79.959	-67.627	24.633
700	12.340	29.270	22.341	4.850	-79.768	-65.583	20.476
800	12.480	30.930	23.318	6.090	-79.586	-63.571	17.367
900	12.620	32.410	24.243	7.350	-79.417	-61.573	14.952
1000	12.750	33.740	25.120	8.620	-79.277	-59.593	13.024
1100	12.880	34.960	25.960	9.900	-79.174	-57.637	11.451
1200	13.020	36.090	26.765	11.190	-79.116	-55.683	10.141
1300	13.160	37.140	27.525	12.500	-79.101	-53.734	9.033
1400	13.290	38.120	28.249	13.820	-79.146	-51.781	8.083
1500	13.420	39.040	28.933	15.160	-79.249	-49.815	7.258
1600	13.560	39.910	29.591	16.510	-79.427	-47.855	6.537
1700	13.700	40.740	30.228	17.870	-79.687	-45.878	5.898
1701	13.701	40.748	30.234	17.884	-79.691	-45.871	5.894
1701	13.701	40.748	30.234	17.884	-80.812	-45.871	5.894
1743	13.756	41.083	30.492	18.460	-80.694	-44.997	5.642
1743	13.756	41.083	30.492	18.460	-83.605	-44.997	5.642
1800	13.830	41.520	30.826	19.250	-83.656	-43.714	5.308
1900	13.960	42.280	31.417	20.640	-83.743	-41.524	4.776
2000	14.100	43.000	31.980	22.040	-83.822	-39.300	4.295

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1701 K, α - β transition point of Ho; ΔH° = 1.121 kcal/mol.
1743 K, melting point of Ho; ΔH° = 2.911 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.400 + 1.350\times10^{-3}T$
$H°-H°_{298} = 11.400\times10^{-3}T + 0.675\times10^{-6}T^2 - 3.459$

Formation equations (kcal/mol):

298.15-1701 K: $\Delta Hf° = -82.297 + 4.800\times10^{-3}T - 1.945\times10^{-6}T^2 + 160.650T^{-1}$
$\Delta Gf° = -82.297 - 4.800\times10^{-3}T\ln T + 1.945\times10^{-6}T^2 + 80.325T^{-1} + 53.711\times10^{-3}T$
1701-1743 K: $\Delta Hf° = -84.340 + 1.441\times10^{-3}T + 0.381\times10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf° = -84.340 - 1.441\times10^{-3}T\ln T - 0.381\times10^{-6}T^2 + 1.975T^{-1} + 33.906\times10^{-3}T$
1743-2000 K: $\Delta Hf° = -80.627 - 2.359\times10^{-3}T + 0.381\times10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf° = -80.627 + 2.359\times10^{-3}T\ln T - 0.381\times10^{-6}T^2 + 1.975T^{-1} + 3.415\times10^{-3}T$

Source: Data from Brown (59, 60) who estimated all except enthalpy of formation at 298 K.

HoO(g)
Holmium Monoxide (ideal gas)
[Formation: $Ho(c,l) + 0.5O_2(g) = HoO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	7.560	61.238	61.238	0	-14.500	-20.107	14.739
300	7.570	61.285	61.238	.014	-14.505	-20.142	14.673
400	7.930	63.512	61.540	.789	-14.743	-21.985	12.012
500	8.200	65.313	62.119	1.597	-14.970	-23.766	10.388
600	8.390	66.826	62.781	2.427	-15.194	-25.506	9.290
700	8.510	68.131	63.455	3.273	-15.412	-27.209	8.495
800	8.600	69.273	64.112	4.129	-15.642	-28.876	7.888
900	8.670	70.291	64.743	4.993	-15.896	-30.513	7.409
1000	8.720	71.207	65.345	5.862	-16.183	-32.125	7.021
1100	8.750	72.040	65.916	6.736	-16.511	-33.710	6.697
1200	8.780	72.803	66.459	7.613	-16.891	-35.249	6.420
1300	8.800	73.506	66.974	8.492	-17.329	-36.763	6.180
1400	8.820	74.159	67.464	9.373	-17.835	-38.236	5.969
1500	8.840	74.768	67.931	10.256	-18.415	-39.672	5.780
1600	8.850	75.340	68.377	11.141	-19.078	-41.079	5.611
1700	8.860	75.876	68.802	12.026	-19.833	-42.424	5.454
1701	8.860	75.881	68.806	12.035	-19.842	-42.450	5.454
1701	8.860	75.881	68.806	12.035	-20.963	-42.450	5.454
1743	8.864	76.097	68.979	12.407	-21.058	-42.966	5.387
1743	8.864	76.097	68.979	12.407	-23.969	-42.966	5.387
1800	8.870	76.382	69.209	12.912	-24.316	-43.578	5.291
1900	8.880	76.863	69.600	13.800	-24.925	-44.648	5.136
2000	8.880	77.318	69.974	14.688	-25.537	-45.666	4.990

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1701 K, α - β transition point of Ho; ΔH° = 1.121 kcal/mol.
1743 K, melting point of Ho; ΔH° = 2.911 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.460 + 0.286\times10^{-3}T - 0.876\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 8.460\times10^{-3}T + 0.143\times10^{-6}T^2 + 0.876\times10^{2}T^{-1} - 2.829$

Formation equations (kcal/mol):

298.15-1701 K: $\Delta Hf^\circ = -15.476 + 1.504\times10^{-3}T - 2.434\times10^{-6}T^2 + 221.700T^{-1}$
$\Delta Gf^\circ = -15.476 - 1.504\times10^{-3}T\ln T + 2.434\times10^{-6}T^2 + 110.850T^{-1} - 8.936\times10^{-3}T$
1701-1743 K: $\Delta Hf^\circ = -17.518 - 1.855\times10^{-3}T - 0.108\times10^{-6}T^2 + 65.000T^{-1}$
$\Delta Gf^\circ = -17.518 + 1.855\times10^{-3}T\ln T + 0.108\times10^{-6}T^2 + 32.500T^{-1} - 28.741\times10^{-3}T$
1743-2000 K: $\Delta Hf^\circ = -13.806 - 5.655\times10^{-3}T - 0.108\times10^{-6}T^2 + 65.000T^{-1}$
$\Delta Gf^\circ = -13.806 + 5.655\times10^{-3}T\ln T + 0.108\times10^{-6}T^2 + 32.500T^{-1} - 59.232\times10^{-3}T$

Source: Data from Pedley (396) who estimated all except enthalpy of formation at 298 K.

InAs(c,l)
Indium Arsenide
[Formation: In(c,l) + As[a,1/4As_4(g)] = InAs(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.380	18.080	18.080	0	-14.000	-12.726	9.328
300	11.396	18.150	18.080	.022	-14.001	-12.717	9.264
400	12.062	21.528	18.538	1.196	-14.091	-12.279	6.709
429.78	12.201	22.399	18.776	1.557	-14.121	-12.143	6.175
429.78	12.201	22.399	18.776	1.557	-14.901	-12.143	6.175
500	12.530	24.272	19.416	2.428	-14.956	-11.685	5.107
600	12.920	26.592	20.425	3.700	-15.013	-11.027	4.016
700	13.272	28.610	21.453	5.010	-15.043	-10.359	3.234
800	13.606	30.404	22.462	6.354	-15.050	-9.689	2.647
876	13.851	31.651	23.207	7.397	-15.041	-9.183	2.291
876	13.851	31.651	23.207	7.397	-23.350	-9.183	2.291
900	13.928	32.026	23.437	7.730	-23.302	-8.796	2.136
1000	14.242	33.510	24.370	9.140	-23.080	-7.195	1.572
1100	14.552	34.882	25.264	10.580	-22.829	-5.617	1.116
1200	14.860	36.160	26.118	12.050	-22.548	-4.064	.740
1210	14.890	36.284	26.202	12.200	-22.517	-3.911	.706
1210	16.000	50.806	26.202	29.770	-4.947	-3.911	.706
1300	16.000	51.952	27.944	31.210	-4.578	-3.846	.647

Phase changes: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
876 K, sublimation point of As to As_4(g); ΔH° = 33.235 kcal/mol of As_4(g).
1210 K, melting point of InAs; ΔH° = 17.570 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1210 K: $Cp° = 11.342 + 2.980\times10^{-3}T - 0.756\times10^{5}T^{-2}$
$H°-H°_{298} = 11.342\times10^{-3}T + 1.490\times10^{-6}T^{2} + 0.756\times10^{2}T^{-1} - 3.768$
1210-1300 K: $Cp° = 16.000$
$H°-H°_{298} = 16.000\times10^{-3}T + 10.410$

Formation equations (kcal/mol):

298.15-429.78 K: $ΔHf° = -15.051 + 3.031\times10^{-3}T - 3.843\times10^{-6}T^{2} + 145.900T^{-1}$
$ΔGf° = -15.051 - 3.031\times10^{-3}T\ln T + 3.843\times10^{-6}T^{2} + 72.950T^{-1} + 23.103\times10^{-3}T$
429.78-876 K: $ΔHf° = -14.692 - 1.316\times10^{-3}T + 0.929\times10^{-6}T^{2} + 80.200T^{-1}$
$ΔGf° = -14.692 + 1.316\times10^{-3}T\ln T - 0.929\times10^{-6}T^{2} + 40.100T^{-1} - 1.862\times10^{-3}T$
876-1210 K: $ΔHf° = -24.020 - 0.618\times10^{-3}T + 1.507\times10^{-6}T^{2} + 48.700T^{-1}$
$ΔGf° = -24.020 + 0.618\times10^{-3}T\ln T - 1.507\times10^{-6}T^{2} + 24.350T^{-1} + 14.043\times10^{-3}T$
1210-1300 K: $ΔHf° = -9.842 + 4.040\times10^{-3}T + 0.017\times10^{-6}T^{2} - 26.900T^{-1}$
$ΔGf° = -9.842 - 4.040\times10^{-3}T\ln T - 0.017\times10^{-6}T^{2} - 13.450T^{-1} + 33.613\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from Piesbergen (400) and Sirota (460). High-temperature data based on Lichter (309).

InH(g)
Indium Hydride (ideal gas)
[Formation: In(c,l) + $0.5H_2(g)$ = InH(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.071	49.607	49.607	0	51.315	45.297	-33.203
300	7.074	49.650	49.607	.013	51.309	45.260	-32.971
400	7.300	51.714	49.887	.731	51.016	43.285	-23.650
429.78	7.382	52.241	50.032	.950	50.921	42.714	-21.720
429.78	7.382	52.241	50.032	.950	50.141	42.714	-21.720
500	7.576	53.372	50.422	1.475	49.927	41.517	-18.147
600	7.837	54.777	51.034	2.246	49.646	39.862	-14.520
700	8.063	56.003	51.659	3.041	49.390	38.252	-11.943
800	8.251	57.092	52.271	3.857	49.155	36.677	-10.020
900	8.406	58.073	52.862	4.690	48.936	35.130	-8.531
1000	8.534	58.966	53.429	5.537	48.729	33.606	-7.345
1100	8.643	59.784	53.969	6.396	48.530	32.105	-6.379
1200	8.735	60.540	54.486	7.265	48.336	30.620	-5.577
1300	8.816	61.243	54.979	8.143	48.146	29.151	-4.901
1400	8.888	61.899	55.450	9.028	47.958	27.698	-4.324
1500	8.953	62.514	55.901	9.920	47.772	26.258	-3.826
1600	9.013	63.094	56.332	10.819	47.587	24.829	-3.391
1700	9.069	63.642	56.746	11.723	47.403	23.414	-3.010
1800	9.123	64.162	57.144	12.632	47.218	22.005	-2.672
1900	9.176	64.657	57.527	13.547	47.035	20.609	-2.371
2000	9.228	65.129	57.895	14.468	46.854	19.223	-2.101

Phase change: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.358 + 1.100\times10^{-3}T - 0.547\times10^{5}T^{-2}$
$H°-H°_{298} = 7.358\times10^{-3}T + 0.550\times10^{-6}T^{2} + 0.547\times10^{2}T^{-1} - 2.426$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = 50.769 + 1.510\times10^{-3}T - 4.421\times10^{-6}T^{2} + 145.650T^{-1}$
$\Delta Gf° = 50.769 - 1.510\times10^{-3}T\ln T + 4.421\times10^{-6}T^{2} + 72.825T^{-1} - 11.887\times10^{-3}T$
429.78-2000 K: $\Delta Hf° = 51.129 - 2.837\times10^{-3}T + 0.350\times10^{-6}T^{2} + 79.950T^{-1}$
$\Delta Gf° = 51.129 + 2.837\times10^{-3}T\ln T - 0.350\times10^{-6}T^{2} + 39.975T^{-1} - 36.853\times10^{-3}T$

Source: Data from Gurvich (196).

InN(c)
Indium Nitride
[Formation: In(c,l) + $0.5N_2(g)$ = InN(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	9.965	10.400	10.400	0	-30.100	-22.257	16.315
300	9.970	10.462	10.402	.018	-30.101	-22.209	16.179
400	10.260	13.370	10.795	1.030	-30.101	-19.580	10.698
429.78	10.346	14.110	10.999	1.337	-30.108	-18.796	9.558
429.78	10.346	14.110	10.999	1.337	-30.888	-18.796	9.558
500	10.550	15.690	11.548	2.071	-30.896	-16.819	7.351
600	10.840	17.639	12.406	3.140	-30.885	-14.005	5.101
700	11.130	19.332	13.276	4.239	-30.850	-11.193	3.495
800	11.420	20.837	14.130	5.366	-30.792	-8.390	2.292
900	11.710	22.199	14.951	6.523	-30.711	-5.593	1.358
1000	12.000	23.448	15.740	7.708	-30.608	-2.809	.614
1100	12.290	24.605	16.493	8.923	-30.482	-.033	.007
1200	12.580	25.687	17.215	10.166	-30.334	2.727	-.497
1300	12.870	26.705	17.906	11.439	-30.162	5.476	-.921
1400	13.160	27.670	18.570	12.740	-29.966	8.210	-1.282
1473	13.372	28.344	19.038	13.708	-29.808	10.197	-1.513

*Data except enthalpy of formation at 298 K and temperature of fusion estimated.

Phase changes: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
1473 K, melting point of InN; ΔH° unknown.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1473 K: $Cp^\circ = 9.100 + 2.900\times10^{-3}T$
$H^\circ - H^\circ_{298} = 9.100\times10^{-3}T + 1.450\times10^{-6}T^2 - 2.842$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf^\circ = -31.031 + 3.222\times10^{-3}T - 3.607\times10^{-6}T^2 + 86.650T^{-1}$
$\Delta Gf^\circ = -31.031 - 3.222\times10^{-3}T\ln T + 3.607\times10^{-6}T^2 + 43.325T^{-1} + 46.218\times10^{-3}T$
429.78-1473 K: $\Delta Hf^\circ = -30.671 - 1.125\times10^{-3}T + 1.166\times10^{-6}T^2 + 20.950T^{-1}$
$\Delta Gf^\circ = -30.671 + 1.125\times10^{-3}T\ln T - 1.166\times10^{-6}T^2 + 10.475T^{-1} + 21.253\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Gordienko (178). Other data from Barin (23) who estimated all except temperature of fusion.

InO(g)
Indium Monoxide (ideal gas)
[Formation: In(c,l) + 0.5O_2(g) = InO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.790	56.831	56.831	0	41.000	35.482	-26.008
300	7.800	56.878	56.831	.014	40.995	35.447	-25.823
400	8.160	59.177	57.142	.814	40.777	33.629	-18.374
429.78	8.228	59.765	57.304	1.058	40.703	33.100	-16.832
429.78	8.228	59.765	57.304	1.058	39.923	33.100	-16.832
500	8.390	61.026	57.740	1.643	39.756	31.998	-13.986
600	8.540	62.570	58.420	2.490	39.524	30.469	-11.098
700	8.630	63.894	59.110	3.349	39.293	28.978	-9.047
800	8.700	65.050	59.781	4.215	39.062	27.519	-7.518
900	8.750	66.078	60.425	5.088	38.833	26.091	-6.336
1000	8.780	67.003	61.038	5.965	38.601	24.686	-5.395
1100	8.810	67.841	61.619	6.844	38.366	23.306	-4.631
1200	8.830	68.608	62.170	7.726	38.129	21.948	-3.997
1300	8.840	69.316	62.693	8.610	37.889	20.608	-3.464
1400	8.860	69.971	63.189	9.495	37.647	19.290	-3.011
1500	8.870	70.583	63.662	10.382	37.404	17.988	-2.621
1600	8.880	71.156	64.113	11.269	37.158	16.700	-2.281
1700	8.880	71.694	64.543	12.157	36.910	15.431	-1.984
1800	8.890	72.203	64.955	13.046	36.660	14.171	-1.721
1900	8.900	72.683	65.349	13.935	36.407	12.930	-1.487
2000	8.900	73.140	65.728	14.825	36.153	11.699	-1.278

Phase change: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.647 + 0.182\times10^{-3}T - 0.810\times10^{5}T^{-2}$

$H°-H°_{298} = 8.647\times10^{-3}T + 0.091\times10^{-6}T^{2} + 0.810\times10^{2}T^{-1} - 2.858$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = 40.245 + 2.412\times10^{-3}T - 4.923\times10^{-6}T^{2} + 141.100T^{-1}$

$\Delta Gf° = 40.245 - 2.412\times10^{-3}T\ln T + 4.923\times10^{-6}T^{2} + 70.550T^{-1} - 4.496\times10^{-3}T$

429.78-2000 K: $\Delta Hf° = 40.605 - 1.935\times10^{-3}T - 0.150\times10^{-6}T^{2} + 75.400T^{-1}$

$\Delta Gf° = 40.605 + 1.935\times10^{-3}T\ln T + 0.150\times10^{-6}T^{2} + 37.700T^{-1} - 29.461\times10^{-3}T$

Source: Data from Pedley (396).

$In_2O(g)$
Diindium Oxide (ideal gas)
[Formation: $2In(c,l) + 0.5O_2(g) = In_2O(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	12.006	71.365	71.365	0	-10.280	-16.011	11.736
300	12.022	71.440	71.367	.022	-10.288	-16.047	11.690
400	12.664	74.994	71.847	1.259	-10.734	-17.904	9.782
429.78	12.777	75.907	72.097	1.638	-10.883	-18.432	9.373
429.78	12.777	75.907	72.097	1.638	-12.443	-18.432	9.373
500	13.045	77.864	72.772	2.546	-12.781	-19.383	8.472
600	13.280	80.265	73.825	3.864	-13.245	-20.658	7.525
700	13.434	82.325	74.896	5.200	-13.698	-21.859	6.825
800	13.538	84.126	75.940	6.549	-14.144	-22.995	6.282
900	13.612	85.725	76.941	7.906	-14.585	-24.075	5.846
1000	13.667	87.162	77.892	9.270	-15.025	-25.106	5.487
1100	13.707	88.467	78.795	10.639	-15.465	-26.092	5.184
1200	13.739	89.661	79.652	12.011	-15.908	-27.040	4.925
1300	13.764	90.761	80.463	13.387	-16.350	-27.949	4.699
1400	13.783	91.782	81.236	14.764	-16.795	-28.823	4.499
1500	13.799	92.733	81.971	16.143	-17.241	-29.664	4.322
1600	13.813	93.625	82.673	17.524	-17.688	-30.481	4.163
1700	13.824	94.462	83.341	18.906	-18.137	-31.263	4.019
1800	13.833	95.253	83.982	20.288	-18.589	-32.028	3.889
1900	13.841	96.001	84.595	21.672	-19.042	-32.761	3.768
2000	13.848	96.711	85.183	23.057	-19.497	-33.472	3.658

Phase change: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.512 + 0.246\times10^{-3}T - 1.404\times10^{5}T^{-2}$

$H°-H°_{298} = 13.512\times10^{-3}T + 0.123\times10^{-6}T^{2} + 1.404\times10^{2}T^{-1} - 4.510$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = -11.760 + 4.657\times10^{-3}T - 9.653\times10^{-6}T^{2} + 283.200T^{-1}$

$\Delta Gf° = -11.760 - 4.657\times10^{-3}T\ln T + 9.653\times10^{-6}T^{2} + 141.600T^{-1} + 7.805\times10^{-3}T$

429.78-2000 K: $\Delta Hf° = -11.041 - 4.037\times10^{-3}T - 0.108\times10^{-6}T^{2} + 151.800T^{-1}$

$\Delta Gf° = -11.041 + 4.037\times10^{-3}T\ln T + 0.108\times10^{-6}T^{2} + 75.900T^{-1} - 42.125\times10^{-3}T$

Source: Data from Gurvich (196).

InOH(g)
Indium Monohydroxide (ideal gas)
[Formation: $In(c,l) + 0.5O_2(g) + 0.5H_2(g) = InOH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.508	59.291	59.291	0	-24.800	-26.400	19.351
300	11.522	59.362	59.292	.021	-24.804	-26.410	19.239
400	12.063	62.760	59.750	1.204	-24.987	-26.918	14.707
429.78	12.149	63.629	59.989	1.565	-25.048	-27.060	13.760
429.78	12.149	63.629	59.989	1.565	-25.828	-27.060	13.760
500	12.353	65.485	60.633	2.426	-25.964	-27.250	11.911
600	12.538	67.755	61.637	3.671	-26.149	-27.490	10.013
700	12.681	69.699	62.653	4.932	-26.328	-27.699	8.648
800	12.812	71.401	63.642	6.207	-26.503	-27.884	7.617
900	12.940	72.917	64.590	7.494	-26.674	-28.046	6.810
1000	13.069	74.287	65.492	8.795	-26.840	-28.189	6.161
1100	13.196	75.539	66.350	10.108	-27.005	-28.316	5.626
1200	13.319	76.692	67.164	11.434	-27.166	-28.428	5.177
1300	13.436	77.763	67.938	12.772	-27.324	-28.527	4.796
1400	13.546	78.763	68.677	14.121	-27.480	-28.613	4.467
1500	13.648	79.701	69.381	15.480	-27.635	-28.689	4.180
1600	13.743	80.585	70.054	16.850	-27.786	-28.755	3.928
1700	13.830	81.421	70.698	18.229	-27.937	-28.809	3.704
1800	13.909	82.213	71.315	19.616	-28.088	-28.857	3.504
1900	13.981	82.967	71.909	21.010	-28.238	-28.896	3.324
2000	14.047	83.686	72.480	22.412	-28.389	-28.927	3.161

Phase change: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.199 + 0.974\times10^{-3}T - 0.872\times10^{5}T^{-2}$

$H°-H°_{298} = 12.199\times10^{-3}T + 0.487\times10^{-6}T^{2} + 0.872\times10^{2}T^{-1} - 3.973$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = -25.716 + 2.736\times10^{-3}T - 4.736\times10^{-6}T^{2} + 155.550T^{-1}$

$\Delta Gf° = -25.716 - 2.736\times10^{-3}T\ln T + 4.736\times10^{-6}T^{2} + 77.775T^{-1} + 11.010\times10^{-3}T$

429.78-2000 K: $\Delta Hf° = -25.357 - 1.611\times10^{-3}T + 0.036\times10^{-6}T^{2} + 89.850T^{-1}$

$\Delta Gf° = -25.357 + 1.611\times10^{-3}T\ln T - 0.036\times10^{-6}T^{2} + 44.925T^{-1} - 13.955\times10^{-3}T$

Source: Data from Gurvich (196).

InP(c)
Indium Phosphide
[Formation: In(c,l) + P(c,l,1/4P_4(g)) = InP(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.880	15.100	15.100	0	-18.900	-16.354	11.988
300	10.899	15.167	15.100	.020	-18.903	-16.339	11.903
317.3	11.011	15.781	15.121	.210	-18.924	-16.189	11.151
317.3	11.011	15.781	15.121	.210	-19.081	-16.189	11.151
400	11.545	18.405	15.538	1.147	-19.216	-15.420	8.425
429.78	11.631	19.237	15.765	1.492	-19.268	-15.136	7.697
429.78	11.631	19.237	15.765	1.492	-20.048	-15.136	7.697
500	11.835	21.016	16.380	2.318	-20.158	-14.323	6.261
550	11.909	22.149	16.855	2.912	-20.231	-13.752	5.464
550	11.909	22.149	16.855	2.912	-23.139	-13.752	5.464
600	11.983	23.188	17.340	3.509	-23.125	-12.898	4.698
700	12.065	25.042	18.311	4.712	-23.094	-11.195	3.495
800	12.111	26.656	19.255	5.921	-23.061	-9.498	2.595
900	12.136	28.084	20.157	7.134	-23.026	-7.803	1.895
910	12.138	28.218	20.246	7.255	-23.023	-7.635	1.834
910	11.707	28.306	20.246	7.335	-22.943	-7.635	1.834
1000	12.292	29.438	21.023	8.415	-22.925	-6.122	1.338
1100	12.943	30.640	21.843	9.677	-22.845	-4.444	.883
1200	13.593	31.794	22.624	11.004	-22.702	-2.778	.506
1300	14.244	32.908	23.373	12.395	-22.496	-1.128	.190

Phase changes:
317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
550 K, boiling point of P to P_4(g); ΔH° = 2.908 kcal/mol of P.
910 K, α - β transition point of InP; ΔH° = 0.080 kcal/mol.
1335 K, melting point of InP; ΔH° = 19.98 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-910 K:
$Cp° = 12.487 - 0.204\times10^{-3}T - 1.375\times10^{5}T^{-2}$
$H°-H°_{298} = 12.487\times10^{-3}T - 0.102\times10^{-6}T^{2} + 1.375\times10^{2}T^{-1} - 4.175$

910-1300 K:
$Cp° = 5.786 + 6.506\times10^{-3}T$
$H°-H°_{298} = 5.786\times10^{-3}T + 3.253\times10^{-6}T^{2} - 0.624$

Formation equations (kcal/mol):

298.15-317.3 K:
$\Delta Hf° = -20.732 + 6.068\times10^{-3}T - 8.049\times10^{-6}T^{2} + 220.200T^{-1}$
$\Delta Gf° = -20.732 - 6.068\times10^{-3}T\ln T + 8.049\times10^{-6}T^{2} + 110.100T^{-1} + 45.620\times10^{-3}T$

317.3-429.78 K:
$\Delta Hf° = -20.419 + 3.575\times10^{-3}T - 4.864\times10^{-6}T^{2} + 220.200T^{-1}$
$\Delta Gf° = -20.419 - 3.575\times10^{-3}T\ln T + 4.864\times10^{-6}T^{2} + 110.100T^{-1} + 31.284\times10^{-3}T$

429.78-550 K:
$\Delta Hf° = -20.059 - 0.772\times10^{-3}T - 0.092\times10^{-6}T^{2} + 154.500T^{-1}$
$\Delta Gf° = -20.059 + 0.772\times10^{-3}T\ln T + 0.092\times10^{-6}T^{2} + 77.250T^{-1} + 6.318\times10^{-3}T$

550-910 K:
$\Delta Hf° = -23.520 + 0.566\times10^{-3}T - 0.096\times10^{-6}T^{2} + 54.200T^{-1}$
$\Delta Gf° = -23.520 - 0.566\times10^{-3}T\ln T + 0.096\times10^{-6}T^{2} + 27.100T^{-1} + 21.216\times10^{-3}T$

910-1300 K:
$\Delta Hf° = -19.969 - 6.135\times10^{-3}T + 3.259\times10^{-6}T^{2} - 83.300T^{-1}$
$\Delta Gf° = -19.969 + 6.135\times10^{-3}T\ln T - 3.259\times10^{-6}T^{2} - 41.650T^{-1} - 25.207\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Tmar (492). Low-temperature heat capacities and entropy at 298 K based on Piesbergen (400) and Sirota (460). High-temperature data based on Pankratz (381). Fusion data from Tmar (492).

$In_2(SO_4)_3(c)$
Indium Sulfate
[Reaction: $2In(c,l) + 1.5S_2(g) + 6O_2(g) = In_2(SO_4)_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	65.704	72.240	72.240	0	-697.405	-598.661	438.825
300	65.972	72.647	72.240	.122	-697.406	-598.046	435.671
400	76.501	93.218	74.973	7.298	-697.015	-564.969	308.681
429.78	78.510	98.784	76.432	9.606	-696.785	-555.146	282.297
429.78	78.510	98.784	76.432	9.606	-698.345	-555.146	282.297
500	83.247	111.051	80.447	15.302	-697.606	-531.800	232.447
600	88.701	126.722	86.880	23.905	-696.208	-498.764	181.672
700	93.716	140.775	93.592	33.028	-694.445	-465.991	145.487
800	98.648	153.610	100.303	42.646	-692.318	-433.500	118.425
900	103.667	165.518	106.896	52.760	-689.799	-401.295	97.446
1000	108.863	176.707	113.322	63.385	-686.857	-369.392	80.730
1100	114.287	187.335	119.570	74.541	-683.468	-337.801	67.114

Phase change: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 66.309 + 43.374x10^{-3}T - 12.033x10^{5}T^{-2}$
$H° - H°_{298} = 66.309x10^{-3}T + 21.687x10^{-6}T^{2} + 12.033x10^{2}T^{-1} - 25.734$

Reaction equations (kcal/mol):

298.15-429.78 K: $ΔHr° = -703.055 + 5.174x10^{-3}T + 8.665x10^{-6}T^{2} + 995.050T^{-1}$
$ΔGr° = -703.055 - 5.174x10^{-3}TlnT - 8.665x10^{-6}T^{2} + 497.525T^{-1} + 376.610x10^{-3}T$
429.78-1100 K: $ΔHr° = -702.336 - 3.520x10^{-3}T + 18.209x10^{-6}T^{2} + 863.650T^{-1}$
$ΔGr° = -702.336 + 3.520x10^{-3}TlnT - 18.209x10^{-6}T^{2} + 431.825T^{-1} + 326.679x10^{-3}T$

Source: Data from DeKock (113).

InSb(c,l)
Indium Antimonide
[Formation: In(c,l) + Sb(c,l) = InSb(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.824	20.600	20.600	0	-7.300	-6.078	4.455
300	11.838	20.674	20.601	.022	-7.301	-6.069	4.421
400	12.390	24.162	21.072	1.236	-7.363	-5.651	3.087
429.78	12.488	25.055	21.317	1.606	-7.388	-5.522	2.808
429.78	12.488	25.055	21.317	1.606	-8.168	-5.522	2.808
500	12.720	26.966	21.982	2.492	-8.218	-5.086	2.223
600	12.964	29.308	23.011	3.778	-8.274	-4.457	1.623
700	13.166	31.320	24.057	5.084	-8.327	-3.813	1.190
797	13.340	33.040	25.047	6.370	-8.383	-3.188	.874
797	16.000	47.356	25.047	17.780	3.027	-3.188	.874
800	16.000	47.418	25.133	17.828	3.033	-3.213	.878
900	16.000	49.302	27.715	19.428	3.217	-4.002	.972
903.9	16.000	49.371	27.809	19.490	3.223	-4.033	.975
903.9	16.000	49.371	27.809	19.490	-1.527	-4.033	.975
1000	16.000	50.988	29.960	21.028	-1.377	-4.312	.942

Phase changes: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
797 K, melting point of InSb; ΔH° = 11.410 kcal/mol.
903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-797 K: $Cp° = 12.363 + 1.394\times10^{-3}T - 0.850\times10^{5}T^{-2}$
$H°-H°_{298} = 12.363\times10^{-3}T + 0.697\times10^{-6}T^{2} + 0.850\times10^{2}T^{-1} - 4.033$
797-1000 K: $Cp° = 16.000$
$H°-H°_{298} = 16.000\times10^{-3}T + 5.028$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = -8.857 + 4.655\times10^{-3}T - 5.237\times10^{-6}T^{2} + 189.300T^{-1}$
$\Delta Gf° = -8.857 - 4.655\times10^{-3}T\ln T + 5.237\times10^{-6}T^{2} + 94.650T^{-1} + 33.219\times10^{-3}T$
429.78-797 K: $\Delta Hf° = -8.498 + 0.308\times10^{-3}T - 0.465\times10^{-6}T^{2} + 123.600T^{-1}$
$\Delta Gf° = -8.498 - 0.308\times10^{-3}T\ln T + 0.465\times10^{-6}T^{2} + 61.800T^{-1} + 8.254\times10^{-3}T$
797-903.9 K: $\Delta Hf° = 0.563 + 3.945\times10^{-3}T - 1.162\times10^{-6}T^{2} + 38.600T^{-1}$
$\Delta Gf° = 0.563 - 3.945\times10^{-3}T\ln T + 1.162\times10^{-6}T^{2} + 19.300T^{-1} + 20.695\times10^{-3}T$
903.9-1000 K: $\Delta Hf° = -2.940 + 1.533\times10^{-3}T + 0.010\times10^{-6}T^{2} + 17.000T^{-1}$
$\Delta Gf° = -2.940 - 1.533\times10^{-3}T\ln T - 0.010\times10^{-6}T^{2} + 8.500T^{-1} + 9.226\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from Piesbergen (400). High-temperature data based on Lichter (308).

InSe(c,l)
Indium Selenide
[Reaction: $In(c,l) + 0.5Se_2(g) = InSe(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	11.750	19.500	19.500	0	-44.850	-37.867	27.757
300	11.760	19.570	19.500	.022	-44.849	-37.823	27.554
400	11.960	22.990	19.962	1.211	-44.822	-35.488	19.390
429.78	11.996	23.850	20.202	1.568	-44.824	-34.793	17.693
429.78	11.996	23.850	20.202	1.568	-45.604	-34.793	17.693
500	12.080	25.680	20.854	2.413	-45.608	-33.030	14.437
600	12.210	27.890	21.845	3.627	-45.601	-30.514	11.115
700	12.350	29.780	22.844	4.855	-45.578	-27.998	8.741
800	12.520	31.440	23.818	6.098	-45.537	-25.488	6.963
900	12.730	32.930	24.751	7.361	-45.472	-22.989	5.582
913	12.760	33.110	24.866	7.527	-45.461	-22.662	5.425
913	14.330	40.700	24.866	14.457	-38.531	-22.662	5.425
1000	14.330	42.010	26.306	15.704	-38.324	-21.166	4.626

Phase changes: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
913 melting point of InSe; ΔH° = 6.930 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-913 K: $Cp^\circ = 11.506 + 1.292\times10^{-3}T - 0.126\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 11.506\times10^{-3}T + 0.646\times10^{-6}T^2 + 0.126\times10^{2}T^{-1} - 3.530$
913-1000 K: $Cp^\circ = 14.330$
$H^\circ - H^\circ_{298} = 14.330\times10^{-3}T + 1.374$

Reaction equations (kcal/mol):

298.15-429.78 K: $\Delta Hr^\circ = -45.777 + 3.554\times10^{-3}T - 3.957\times10^{-6}T^2 + 65.350T^{-1}$
$\Delta Gr^\circ = -45.777 - 3.554\times10^{-3}T\ln T + 3.957\times10^{-6}T^2 + 32.675T^{-1} + 45.232\times10^{-3}T$
429.78-913 K: $\Delta Hr^\circ = -45.417 - 0.793\times10^{-3}T + 0.816\times10^{-6}T^2 - 0.350T^{-1}$
$\Delta Gr^\circ = -45.417 + 0.793\times10^{-3}T\ln T - 0.816\times10^{-6}T^2 - 0.175T^{-1} + 20.266\times10^{-3}T$
913-1000 K: $\Delta Hr^\circ = -40.513 + 2.031\times10^{-3}T + 0.169\times10^{-6}T^2 - 12.950T^{-1}$
$\Delta Gr^\circ = -40.513 - 2.031\times10^{-3}T\ln T - 0.169\times10^{-6}T^2 - 6.475T^{-1} + 33.563\times10^{-3}T$

Source: Data from Mills (332, 333).

$In_2Se(g)$
Diindium Selenide (ideal gas)
[Reaction: $2In(c,l) + 0.5Se_2(g) = In_2Se(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°$_{298}$)/T	H°- H°$_{298}$	ΔHr°	ΔGr°	
298.15	13.596	79.669	79.669	0	21.850	15.014	-11.005
300	13.597	79.754	79.671	.025	21.842	14.971	-10.906
400	13.730	83.686	80.203	1.393	21.385	12.745	-6.963
429.78	13.749	84.673	80.479	1.802	21.224	12.108	-6.157
429.78	13.749	84.673	80.479	1.802	19.664	12.108	-6.157
500	13.794	86.757	81.219	2.769	19.289	10.903	-4.765
600	13.829	89.276	82.359	4.150	18.760	9.273	-3.378
700	13.850	91.409	83.503	5.534	18.239	7.735	-2.415
800	13.864	93.259	84.609	6.920	17.725	6.271	-1.713
900	13.874	94.893	85.663	8.307	17.218	4.869	-1.182
1000	13.881	96.355	86.660	9.695	16.716	3.522	-.770
1100	13.886	97.678	87.603	11.083	16.217	2.230	-.443
1200	13.890	98.887	88.494	12.472	15.722	.978	-.178
1300	13.893	99.999	89.337	13.861	15.230	-.230	.039
1400	13.895	101.028	90.134	15.251	14.742	-1.399	.218
1500	13.897	101.987	90.894	16.640	14.255	-2.535	.369
1600	13.899	102.884	91.615	18.030	13.773	-3.642	.497
1700	13.900	103.727	92.303	19.420	13.293	-4.707	.605
1800	13.901	104.521	92.960	20.810	12.816	-5.760	.699
1900	13.902	105.273	93.589	22.200	12.343	-6.781	.780
2000	13.903	105.986	94.191	23.590	11.873	-7.779	.850

Phase change: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.899 + 0.008\times10^{-3}T - 0.272\times10^{5}T^{-2}$
$H° - H°_{298} = 13.899\times10^{-3}T + 0.004\times10^{-6}T^{2} + 0.272\times10^{2}T^{-1} - 4.236$

Reaction equations (kcal/mol):

298.15-429.78 K: $\Delta Hr° = 21.145 + 3.327\times10^{-3}T - 9.361\times10^{-6}T^{2} + 162.650T^{-1}$
$\Delta Gr° = 21.145 - 3.327\times10^{-3}T\ln T + 9.361\times10^{-6}T^{2} + 81.325T^{-1} - 5.313\times10^{-3}T$
429.78-2000 K: $\Delta Hr° = 21.864 - 5.367\times10^{-3}T + 0.184\times10^{-6}T^{2} + 31.250T^{-1}$
$\Delta Gr° = 21.864 + 5.367\times10^{-3}T\ln T - 0.184\times10^{-6}T^{2} + 15.625T^{-1} - 55.243\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (332). Other data from Greenberg (182).

$In_2Se_3(c)$
Diindium Triselenide
[Reaction: $2In(c,l) + 1.5Se_2(g) = In_2Se_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	30.000	48.330	48.330	0	-126.950	-107.090	78.498
300	30.040	48.520	48.337	.055	-126.946	-106.969	77.926
350	30.240	53.140	48.691	1.557	-126.837	-103.648	64.720
400	30.850	57.220	49.510	3.084	-126.738	-100.343	54.824
429.78	31.261	59.446	50.120	4.008	-126.682	-98.379	50.026
429.78	31.261	59.446	50.120	4.008	-128.242	-98.379	50.026
450	31.540	60.890	50.572	4.643	-128.199	-96.974	47.096
486	32.110	63.340	51.425	5.790	-128.103	-94.477	42.485
486	31.290	65.230	51.425	6.710	-127.183	-94.477	42.485
500	31.410	66.130	51.832	7.149	-127.152	-93.540	40.886
550	31.840	69.140	53.267	8.730	-127.032	-90.185	35.836
600	32.270	71.930	54.710	10.332	-126.890	-86.843	31.632
650	32.700	74.530	56.136	11.956	-126.724	-83.510	28.078
700	33.130	76.970	57.539	13.602	-126.535	-80.193	25.037

Phase changes: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
486 K, α - β transition point of In_2Se_3; ΔH° = 0.920 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-486 K: $Cp° = 19.180 + 23.928\times10^{-3}T + 3.277\times10^{5}T^{-2}$
$H°- H°_{298} = 19.180\times10^{-3}T + 11.964\times10^{-6}T^{2} - 3.277\times10^{2}T^{-1} - 5.683$
486-700 K: $Cp° = 27.004 + 8.710\times10^{-3}T + 0.126\times10^{5}T^{-2}$
$H°- H°_{298} = 27.004\times10^{-3}T + 4.355\times10^{-6}T^{2} - 0.126\times10^{2}T^{-1} - 7.417$

Reaction equations (kcal/mol):

298.15-429.78 K: $\Delta Hr° = -125.751 - 2.056\times10^{-3}T + 2.918\times10^{-6}T^{2} - 252.150T^{-1}$
$\Delta Gr° = -125.751 + 2.056\times10^{-3}T\ln T - 2.918\times10^{-6}T^{2} - 126.075T^{-1} + 53.162\times10^{-3}T$
429.78-486 K: $\Delta Hr° = -125.031 - 10.750\times10^{-3}T + 12.463\times10^{-6}T^{2} - 383.550T^{-1}$
$\Delta Gr° = -125.031 + 10.750\times10^{-3}T\ln T - 12.463\times10^{-6}T^{2} - 191.775T^{-1} + 3.231\times10^{-3}T$
486-700 K: $\Delta Hr° = -126.765 - 2.926\times10^{-3}T + 4.853\times10^{-6}T^{2} - 68.450T^{-1}$
$\Delta Gr° = -126.765 + 2.926\times10^{-3}T\ln T - 4.853\times10^{-6}T^{2} - 34.225T^{-1} + 50.834\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Vendrikh (509). Low-temperature heat capacities and entropy at 298 K from Koshchenko (284). High-temperature data from Mills (333).

InTe(c,l)
Indium Telluride
[Reaction: In(c,l) + $0.5Te_2(g)$ = InTe(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15	11.410	25.260	25.260	0	-36.365	-30.553	22.395
300*	11.420	25.330	25.260	.021	-36.364	-30.517	22.231
400	11.880	28.680	25.715	1.186	-36.303	-28.579	15.615
429.78	12.017	29.538	25.951	1.542	-36.289	-28.005	14.241
429.78	12.017	29.538	25.951	1.542	-37.069	-28.005	14.241
500	12.340	31.380	26.584	2.398	-37.023	-26.525	11.594
600	12.810	33.670	27.578	3.655	-36.924	-24.432	8.899
700	13.270	35.680	28.596	4.959	-36.785	-22.362	6.982
800	13.730	37.480	29.593	6.310	-36.605	-20.312	5.549
900	14.200	39.130	30.568	7.706	-36.385	-18.294	4.442
965	14.500	40.130	31.176	8.640	-36.220	-16.992	3.848
965	14.500	49.020	31.176	17.220	-27.640	-16.992	3.848
1000	14.500	49.540	31.813	17.727	-27.548	-16.610	3.630
1100	14.500	50.920	33.486	19.177	-27.290	-15.524	3.084
1200	14.500	52.180	34.991	20.627	-27.040	-14.463	2.634

*Data above 298 K except temperature and enthalpy of fusion estimated.

Phase changes: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
965 K, melting point of InTe; ΔH° = 8.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-965 K: $Cp^\circ = 10.032 + 4.630\times10^{-3}T$
$H^\circ - H^\circ_{298} = 10.032\times10^{-3}T + 2.315\times10^{-6}T^2 - 3.197$
965-1200 K: $Cp^\circ = 14.498$
$H^\circ - H^\circ_{298} = 14.498\times10^{-3}T + 3.229$

Reaction equations (kcal/mol):

298.15-429.78 K: $\Delta Hr^\circ = -37.286 + 3.112\times10^{-3}T - 2.743\times10^{-6}T^2 + 70.600T^{-1}$
$\Delta Gr^\circ = -37.286 - 3.112\times10^{-3}T\ln T + 2.743\times10^{-6}T^2 + 35.300T^{-1} + 39.102\times10^{-3}T$
429.78-965 K: $\Delta Hr^\circ = -36.926 - 1.235\times10^{-3}T + 2.028\times10^{-6}T^2 + 4.900T^{-1}$
$\Delta Gr^\circ = -36.926 + 1.235\times10^{-3}T\ln T - 2.028\times10^{-6}T^2 + 2.450T^{-1} + 14.137\times10^{-3}T$
965-1200 K: $\Delta Hr^\circ = -30.500 + 3.231\times10^{-3}T - 0.286\times10^{-6}T^2 + 4.900T^{-1}$
$\Delta Gr^\circ = -30.500 - 3.231\times10^{-3}T\ln T + 0.286\times10^{-6}T^2 + 2.450T^{-1} + 35.935\times10^{-3}T$

Source: Data from Mills (332) who estimated all above 298 K except temperature and enthalpy of fusion.

IrO(g)
Iridium Monoxide (ideal gas)
[Formation: Ir(c) + $0.5O_2$(g) = IrO(g)]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.510	59.284	59.284	0	120.500	112.659	-82.580
300	7.510	59.330	59.284	.014	120.496	112.610	-82.035
400	7.850	61.536	59.583	.781	120.303	110.010	-60.106
500	8.140	63.321	60.157	1.582	120.123	107.459	-46.970
600	8.350	64.824	60.812	2.407	119.940	104.943	-38.225
700	8.490	66.123	61.482	3.249	119.751	102.457	-31.988
800	8.600	67.264	62.134	4.104	119.550	100.000	-27.318
900	8.680	68.281	62.761	4.968	119.336	97.570	-23.693
1000	8.740	69.199	63.360	5.839	119.108	95.164	-20.798
1100	8.780	70.034	63.929	6.715	118.865	92.781	-18.434
1200	8.820	70.800	64.471	7.595	118.605	90.420	-16.468
1300	8.850	71.508	64.986	8.479	118.332	88.081	-14.808
1400	8.880	72.165	65.475	9.366	118.042	85.766	-13.389
1500	8.900	72.778	65.941	10.256	117.737	83.472	-12.162
1600	8.920	73.354	66.387	11.147	117.415	81.197	-11.091
1700	8.940	73.895	66.812	12.041	117.077	78.946	-10.149
1800	8.960	74.407	67.220	12.936	116.721	76.712	-9.314
1900	8.970	74.892	67.612	13.832	116.347	74.499	-8.569
2000	8.990	75.352	67.987	14.730	115.956	72.307	-7.901

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.276 + 0.464\text{x}10^{-3}T - 0.804\text{x}10^{5}T^{-2}$

$H°-H°_{298} = 8.276\text{x}10^{-3}T + 0.232\text{x}10^{-6}T^{2} + 0.804\text{x}10^{2}T^{-1} - 2.758$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 120.576 - 0.787\text{x}10^{-3}T - 0.758\text{x}10^{-6}T^{2} + 67.400T^{-1}$

$\Delta Gf° = 120.576 + 0.787\text{x}10^{-3}T\ln T + 0.758\text{x}10^{-6}T^{2} + 33.700T^{-1} - 31.645\text{x}10^{-3}T$

Source: Data from Pedley (396).

$IrO_2(c)$
Iridium Dioxide
[Formation: $Ir(c) + O_2(g) = IrO_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.300	12.192	12.192	0	-59.600	-46.096	33.789
300	13.345	12.274	12.192	.025	-59.599	-46.011	33.519
400	15.104	16.380	12.740	1.456	-59.483	-41.496	22.672
500	16.180	19.874	13.826	3.024	-59.262	-37.022	16.182
600	16.988	22.898	15.093	4.683	-58.988	-32.601	11.875
700	17.668	25.569	16.402	6.417	-58.675	-28.227	8.813
800	18.281	27.968	17.699	8.215	-58.332	-23.901	6.529
900	18.854	30.155	18.964	10.072	-57.960	-19.618	4.764
1000	19.403	32.170	20.185	11.985	-57.559	-15.379	3.361
1100	19.936	34.044	21.360	13.952	-57.131	-11.181	2.221
1200	20.458	35.802	22.492	15.972	-56.674	-7.025	1.279

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 14.791 + 4.874\times10^{-3}T - 2.619\times10^{5}T^{-2}$

$H°- H°_{298} = 14.791\times10^{-3}T + 2.437\times10^{-6}T^{2} + 2.619\times10^{2}T^{-1} - 5.505$

Formation equations (kcal/mol):

298.15-1200 K: $\Delta Hf° = -61.095 + 2.113\times10^{-3}T + 1.195\times10^{-6}T^{2} + 226.300T^{-1}$

$\Delta Gf° = -61.095 - 2.113\times10^{-3}T\ln T - 1.195\times10^{-6}T^{2} + 113.150T^{-1} + 61.431\times10^{-3}T$

Source: Data based on Cordfunke (97).

K_3AlF_6(c,l)
Tripotassium Hexafluoroaluminate
[Formation: $3K(c,l,g) + Al(c,l) + 3F_2(g) = K_3AlF_6(c,l)$]

T,K	cal/mol·K Cp°	S°	-(G°- H°_{298})/T	kcal/mol H°- H°_{298}	ΔHf°	ΔGf°	Log Kf
298.15*	53.250	68.000	68.000	0	-786.500	-747.599	547.997
300	53.390	68.330	68.000	.099	-786.493	-747.357	544.443
336.35	54.928	74.524	68.377	2.068	-786.376	-742.623	482.527
336.35	54.928	74.524	68.377	2.068	-788.050	-742.623	482.527
400	57.620	84.425	70.165	5.704	-787.735	-734.055	401.064
500	61.020	97.657	74.377	11.640	-787.064	-720.707	315.017
600	63.910	109.046	79.228	17.891	-786.132	-707.518	257.710
700	66.660	119.105	84.219	24.420	-784.977	-694.503	216.831
800	69.330	128.182	89.157	31.220	-783.618	-681.673	186.222
900	71.400	136.472	93.960	38.261	-782.086	-669.016	162.457
933.61	71.938	139.100	95.538	40.670	-781.550	-664.804	155.623
933.61	71.938	139.100	95.538	40.670	-784.130	-664.804	155.623
1000	73.000	144.081	98.597	45.484	-783.016	-656.362	143.446
1043.7	73.612	147.216	100.568	48.687	-782.260	-650.841	136.284
1043.7	73.612	147.216	100.568	48.687	-839.374	-650.841	136.284
1100	74.400	151.106	103.055	52.856	-837.972	-640.707	127.295
1200	75.600	157.633	107.335	60.358	-835.393	-622.885	113.441
1273	76.330	162.120	110.352	65.900	-833.449	-610.018	104.727
1273	93.800	185.136	110.352	95.200	-804.149	-610.018	104.727
1300	93.800	187.105	111.926	97.733	-802.950	-605.913	101.862
1400	93.800	194.056	117.547	107.113	-798.520	-590.922	92.246
1500	93.800	200.528	122.866	116.493	-794.099	-576.249	83.958

*Data estimated except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

Phase changes:
336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1273 K, melting point of K_3AlF_6; ΔH° = 29.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1273 K: $Cp^\circ = 55.435 + 17.712\times10^{-3}T - 6.635\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 55.435\times10^{-3}T + 8.856\times10^{-6}T^2 + 6.635\times10^{2}T^{-1} - 19.541$
1273-1500 K: $Cp^\circ = 93.800$
$H^\circ - H^\circ_{298} = 93.800\times10^{-3}T - 24.207$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -792.288 + 22.181\times10^{-3}T - 23.597\times10^{-6}T^2 + 379.400T^{-1}$
$\Delta Gf^\circ = -792.288 - 22.181\times10^{-3}T\ln T + 23.597\times10^{-6}T^2 + 189.700T^{-1} + 267.099\times10^{-3}T$
336.35-933.61 K: $\Delta Hf^\circ = -792.279 + 4.784\times10^{-3}T + 6.259\times10^{-6}T^2 + 645.200T^{-1}$
$\Delta Gf^\circ = -792.279 - 4.784\times10^{-3}T\ln T - 6.259\times10^{-6}T^2 + 322.600T^{-1} + 174.719\times10^{-3}T$
933.61-1043.7 K: $\Delta Hf^\circ = -793.546 + 1.786\times10^{-3}T + 7.986\times10^{-6}T^2 + 627.800T^{-1}$
$\Delta Gf^\circ = -793.546 - 1.786\times10^{-3}T\ln T - 7.986\times10^{-6}T^2 + 313.900T^{-1} + 157.196\times10^{-3}T$
1043.7-1273 K: $\Delta Hf^\circ = -858.355 + 8.800\times10^{-3}T + 7.968\times10^{-6}T^2 + 1038.800T^{-1}$
$\Delta Gf^\circ = -858.355 - 8.800\times10^{-3}T\ln T - 7.968\times10^{-6}T^2 + 519.400T^{-1} + 267.835\times10^{-3}T$
1273-1500 K: $\Delta Hf^\circ = -863.021 + 47.165\times10^{-3}T - 0.888\times10^{-6}T^2 + 375.300T^{-1}$
$\Delta Gf^\circ = -863.021 - 47.165\times10^{-3}T\ln T + 0.888\times10^{-6}T^2 + 187.650T^{-1} + 534.707\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Temperature and enthalpy of fusion from Holm (209). Other data are those estimated by JANAF (127).

$KAlO_2(c)$
Potassium Aluminate
[Formation: $K(c,l,g) + Al(c,l) + O_2(g) = KAlO_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	18.193	20.448	20.448	0	-272.521	-257.378	188.661
300	18.246	20.561	20.448	.034	-272.524	-257.284	187.429
336.35	19.103	22.697	20.578	.713	-272.586	-255.434	165.971
336.35	19.103	22.697	20.578	.713	-273.144	-255.434	165.971
400	20.604	26.164	21.196	1.987	-273.193	-252.078	137.727
500	22.225	30.944	22.680	4.132	-273.146	-246.801	107.875
600	23.488	35.112	24.412	6.420	-272.990	-241.544	87.981
700	24.511	38.812	26.209	8.822	-272.764	-236.319	73.781
800	25.342	42.141	27.996	11.316	-272.499	-231.133	63.142
810	25.416	42.457	28.173	11.570	-272.471	-230.616	62.223
810	24.304	42.840	28.173	11.880	-272.161	-230.616	62.223
900	24.563	45.414	29.771	14.079	-272.022	-226.008	54.881
933.61	24.659	46.316	30.350	14.906	-271.978	-224.290	52.504
933.61	24.659	46.316	30.350	14.906	-274.558	-224.290	52.504
1000	24.849	48.017	31.467	16.550	-274.449	-220.720	48.238
1043.7	24.974	49.083	32.182	17.639	-274.376	-218.373	45.726
1043.7	24.974	49.083	32.182	17.639	-293.414	-218.373	45.726
1100	25.136	50.399	33.082	19.049	-293.185	-214.331	42.583
1200	25.423	52.598	34.617	21.577	-292.761	-207.179	37.732
1300	25.710	54.644	36.079	24.134	-292.315	-200.066	33.634
1400	25.997	56.560	37.475	26.719	-291.850	-192.986	30.126

Phase changes:
336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
810 K, α - β transition point of $KAlO_2$; ΔH° = 0.310 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-810 K:
$Cp° = 19.369 + 8.256 \times 10^{-3}T - 3.233 \times 10^{5}T^{-2}$
$H° - H°_{298} = 19.369 \times 10^{-3}T + 4.128 \times 10^{-6}T^{2} + 3.233 \times 10^{2}T^{-1} - 7.226$

810-1400 K:
$Cp° = 21.976 + 2.874 \times 10^{-3}T + 0.001 \times 10^{5}T^{-2}$
$H° - H°_{298} = 21.976 \times 10^{-3}T + 1.437 \times 10^{-6}T^{2} - 0.001 \times 10^{2}T^{-1} - 6.863$

Formation equations (kcal/mol):

298.15-336.35 K:
$\Delta Hf° = -274.724 + 6.501 \times 10^{-3}T - 8.170 \times 10^{-6}T^{2} + 295.500T^{-1}$
$\Delta Gf° = -274.724 - 6.501 \times 10^{-3}T\ln T + 8.170 \times 10^{-6}T^{2} + 147.750T^{-1} + 91.121 \times 10^{-3}T$

336.35-810 K:
$\Delta Hf° = -274.721 + 0.702 \times 10^{-3}T + 1.782 \times 10^{-6}T^{2} + 384.100T^{-1}$
$\Delta Gf° = -274.721 - 0.702 \times 10^{-3}T\ln T - 1.782 \times 10^{-6}T^{2} + 192.050T^{-1} + 60.328 \times 10^{-3}T$

810-933.61 K:
$\Delta Hf° = -274.358 + 3.309 \times 10^{-3}T - 0.909 \times 10^{-6}T^{2} + 60.700T^{-1}$
$\Delta Gf° = -274.358 - 3.309 \times 10^{-3}T\ln T + 0.909 \times 10^{-6}T^{2} + 30.350T^{-1} + 75.406 \times 10^{-3}T$

933.61-1043.7 K:
$\Delta Hf° = -275.625 + 0.311 \times 10^{-3}T + 0.818 \times 10^{-6}T^{2} + 43.300T^{-1}$
$\Delta Gf° = -275.625 - 0.311 \times 10^{-3}T\ln T - 0.818 \times 10^{-6}T^{2} + 21.650T^{-1} + 57.882 \times 10^{-3}T$

1043.7-1400 K:
$\Delta Hf° = -297.228 + 2.649 \times 10^{-3}T + 0.812 \times 10^{-6}T^{2} + 180.300T^{-1}$
$\Delta Gf° = -297.228 - 2.649 \times 10^{-3}T\ln T - 0.812 \times 10^{-6}T^{2} + 90.150T^{-1} + 94.762 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Bennington (32). Other data from Beyer (41).

$KAl(SO_4)_2(c)$
Potassium Aluminum Sulfate
[Reaction: $K(c,l,g) + Al(c,l) + S_2(g) + 4O_2(g) = KAl(SO_4)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	46.141	48.940	48.940	0	-621.270	-554.538	406.482
300	46.776	49.229	48.942	.086	-621.274	-554.123	403.673
336.35	49.844	54.754	49.278	1.842	-621.314	-545.985	354.760
336.35	49.844	54.754	49.278	1.842	-621.872	-545.985	354.760
400	55.217	63.975	50.895	5.232	-621.678	-531.641	290.471
500	60.184	76.867	54.829	11.019	-621.009	-509.199	222.568
600	63.782	88.171	59.463	17.225	-620.048	-486.921	177.359
700	66.735	98.231	64.297	23.754	-618.890	-464.823	145.122
800	69.343	107.315	69.115	30.560	-617.578	-442.905	120.995
900	71.751	115.623	73.827	37.616	-616.130	-421.157	102.269
933.61	72.519	118.268	75.380	40.040	-615.616	-413.885	96.886
933.61	72.519	118.268	75.380	40.040	-618.196	-413.885	96.886
1000	74.035	123.302	78.396	44.906	-617.106	-399.395	87.287
1043.7	74.998	126.489	80.343	48.162	-616.351	-389.896	81.643
1043.7	74.998	126.489	80.343	48.162	-635.389	-389.896	81.643
1100	76.238	130.462	82.807	52.421	-634.238	-376.682	74.839

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 56.769 + 18.534\times10^{-3}T - 14.359\times10^{5}T^{-2}$
$H°- H°_{298} = 56.769\times10^{-3}T + 9.267\times10^{-6}T^{2} + 14.359\times10^{2}T^{-1} - 22.565$

Reaction equations (kcal/mol):

298.15-336.35 K: $\Delta Hr° = -629.012 + 13.868\times10^{-3}T - 4.860\times10^{-6}T^{2} + 1204.200T^{-1}$
$\Delta Gr° = -629.012 - 13.868\times10^{-3}T\ln T + 4.860\times10^{-6}T^{2} + 602.100T^{-1} + 320.577\times10^{-3}T$
336.35-933.61 K: $\Delta Hr° = -629.008 + 8.069\times10^{-3}T + 5.092\times10^{-6}T^{2} + 1292.800T^{-1}$
$\Delta Gr° = -629.008 - 8.069\times10^{-3}T\ln T - 5.092\times10^{-6}T^{2} + 646.400T^{-1} + 289.783\times10^{-3}T$
933.61-1043.7 K: $\Delta Hr° = -630.276 + 5.071\times10^{-3}T + 6.819\times10^{-6}T^{2} + 1275.400T^{-1}$
$\Delta Gr° = -630.276 - 5.071\times10^{-3}T\ln T - 6.819\times10^{-6}T^{2} + 637.700T^{-1} + 272.260\times10^{-3}T$
1043.7-1100 K: $\Delta Hr° = -651.879 + 7.409\times10^{-3}T + 6.813\times10^{-6}T^{2} + 1412.400T^{-1}$
$\Delta Gr° = -651.879 - 7.409\times10^{-3}T\ln T - 6.813\times10^{-6}T^{2} + 706.200T^{-1} + 309.139\times10^{-3}T$

Source: Data from DeKock (113).

$KAlSiO_4(c)$
Potassium Aluminum Silicate, Kaliophilite
[Formation: $K(c,l,g) + Al(c,l) + Si(c,l) + 2O_2(g) = KAlSiO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	28.630	31.850	31.850	0	-503.900	-476.204	349.062
300	28.725	32.027	31.850	.053	-503.906	-476.032	346.784
336.35	30.258	35.400	32.055	1.125	-504.009	-472.649	307.109
336.35	30.258	35.400	32.055	1.125	-504.567	-472.649	307.109
400	32.943	40.902	33.032	3.148	-504.650	-466.602	254.936
500	36.081	48.605	35.393	6.606	-504.567	-457.093	199.792
600	38.565	55.411	38.173	10.343	-504.289	-447.620	163.043
700	40.550	61.511	41.080	14.302	-503.875	-438.207	136.813
800	42.101	67.032	43.984	18.438	-503.371	-428.861	117.158
810	42.233	67.555	44.271	18.860	-503.317	-427.929	115.460
810	42.500	67.759	44.271	19.025	-503.152	-427.929	115.460
900	42.500	72.237	46.848	22.850	-502.679	-419.597	101.891
933.61	42.500	73.795	47.790	24.278	-502.520	-416.498	97.497
933.61	42.500	73.795	47.790	24.278	-505.100	-416.498	97.497
1000	42.500	76.715	49.615	27.100	-504.782	-410.201	89.648
1043.7	42.500	78.533	50.788	28.957	-504.583	-406.071	85.030
1043.7	42.500	78.533	50.788	28.957	-523.621	-406.071	85.030
1100	42.500	80.765	52.265	31.350	-523.243	-399.747	79.421
1200	42.500	84.463	54.796	35.600	-522.589	-388.548	70.763
1300	42.500	87.865	57.211	39.850	-521.956	-377.405	63.447
1400	42.500	91.015	59.515	44.100	-521.347	-366.304	57.182
1500	42.500	93.947	61.714	48.350	-520.756	-355.262	51.761
1600	42.500	96.690	63.815	52.600	-520.185	-344.251	47.022
1687	42.500	98.940	65.568	56.297	-519.700	-334.675	43.356
1687	42.500	98.940	65.568	56.297	-531.782	-334.675	43.356
1700	42.500	99.266	65.825	56.850	-531.702	-333.152	42.829
1800	42.500	101.696	67.752	61.100	-531.096	-321.488	39.033

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
810 K, α - β transition point of $KAlSiO_4$; ΔH° = 0.165 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-810 K: $Cp° = 29.570 + 17.156\times10^{-3}T - 5.383\times10^{5}T^{-2}$
$H°-H°_{298} = 29.570\times10^{-3}T + 8.578\times10^{-6}T^{2} + 5.383\times10^{2}T^{-1} - 11.384$
810-1800 K: $Cp° = 42.500$
$H°-H°_{298} = 42.500\times10^{-3}T - 15.400$

Formation equations (kcal/mol):

298.15-336.35 K: $ΔHf° = -505.855 + 3.793\times10^{-3}T - 4.574\times10^{-6}T^{2} + 366.800T^{-1}$
$ΔGf° = -505.855 - 3.793\times10^{-3}T\ln T + 4.574\times10^{-6}T^{2} + 183.400T^{-1} + 117.633\times10^{-3}T$
336.35-810 K: $ΔHf° = -505.851 - 2.006\times10^{-3}T + 5.378\times10^{-6}T^{2} + 455.400T^{-1}$
$ΔGf° = -505.851 + 2.006\times10^{-3}T\ln T - 5.378\times10^{-6}T^{2} + 227.700T^{-1} + 86.840\times10^{-3}T$
810-933.61 K: $ΔHf° = -509.867 + 10.924\times10^{-3}T - 3.200\times10^{-6}T^{2} - 82.900T^{-1}$
$ΔGf° = -509.867 - 10.924\times10^{-3}T\ln T + 3.200\times10^{-6}T^{2} - 41.450T^{-1} + 171.852\times10^{-3}T$
933.61-1043.7 K: $ΔHf° = -511.135 + 7.926\times10^{-3}T - 1.473\times10^{-6}T^{2} - 100.300T^{-1}$
$ΔGf° = -511.135 - 7.926\times10^{-3}T\ln T + 1.473\times10^{-6}T^{2} - 50.150T^{-1} + 154.329\times10^{-3}T$
1043.7-1687 K: $ΔHf° = -532.738 + 10.264\times10^{-3}T - 1.479\times10^{-6}T^{2} + 36.700T^{-1}$
$ΔGf° = -532.738 - 10.264\times10^{-3}T\ln T + 1.479\times10^{-6}T^{2} + 18.350T^{-1} + 191.208\times10^{-3}T$
1687-1800 K: $ΔHf° = -545.167 + 9.843\times10^{-3}T - 1.128\times10^{-6}T^{2} + 135.200T^{-1}$
$ΔGf° = -545.167 - 9.843\times10^{-3}T\ln T + 1.128\times10^{-6}T^{2} + 67.600T^{-1} + 196.022\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Barany (20). Low-temperature heat capacities and entropy at 298 K from Kelley (250). High-temperature data based on Pankratz (382).

$KAlSi_2O_6(c)$
Potassium Aluminum Disilicate, Leucite
[Formation: $K(c,l,g) + Al(c,l) + 2Si(c,l) + 3O_2(g) = KAlSi_2O_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	39.230	47.850	47.850	0	-721.700	-682.822	500.515
300	39.365	48.094	47.851	.073	-721.708	-682.580	497.253
336.35	41.512	52.719	48.132	1.543	-721.847	-677.831	440.428
336.35	41.512	52.719	48.132	1.543	-722.405	-677.831	440.428
400	45.272	60.269	49.469	4.320	-722.517	-669.388	365.732
500	49.602	70.858	52.712	9.073	-722.416	-656.108	286.781
600	53.134	80.221	56.531	14.214	-722.061	-642.876	234.164
700	56.479	88.661	60.528	19.693	-721.496	-629.721	196.605
800	60.177	96.438	64.537	25.521	-720.703	-616.662	168.462
900	64.736	103.778	68.491	31.758	-719.620	-603.717	146.601
933.61	66.603	106.183	69.805	33.963	-719.172	-599.397	140.312
933.61	66.603	106.183	69.805	33.963	-721.752	-599.397	140.312
955	67.792	107.705	70.637	35.400	-721.429	-596.582	136.525
955	56.211	107.705	70.637	35.400	-721.429	-596.582	136.525
1000	56.370	110.297	72.364	37.933	-721.253	-590.704	129.097
1043.7	56.525	112.711	74.003	40.400	-721.087	-585.002	122.497
1043.7	56.525	112.711	74.003	40.400	-740.125	-585.002	122.497
1100	56.724	115.687	76.062	43.588	-739.785	-576.658	114.570
1200	57.079	120.637	79.572	49.278	-739.183	-561.853	102.326
1300	57.433	125.220	82.909	55.004	-738.580	-547.102	91.975
1400	57.787	129.489	86.085	60.765	-737.981	-532.385	83.108
1500	58.142	133.488	89.114	66.561	-737.377	-517.746	75.435
1600	58.496	137.252	92.006	72.393	-736.769	-503.127	68.723
1687	58.804	140.357	94.421	77.495	-736.232	-490.395	63.530
1687	58.804	140.357	94.421	77.495	-760.396	-490.395	63.530
1700	58.850	140.809	94.774	78.260	-760.298	-488.307	62.775
1800	59.205	144.183	97.426	84.163	-759.537	-472.322	57.347

Phase changes:
336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
955 K, α - β transition point of $KAlSi_2O_6$; ΔH° = 0 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-955 K: $Cp° = 34.448 + 33.652\times10^{-3}T - 4.668\times10^{5}T^{-2}$
$H°-H°_{298} = 34.448\times10^{-3}T + 16.826\times10^{-6}T^{2} + 4.668\times10^{2}T^{-1} - 13.332$
955-1800 K: $Cp° = 52.826 + 3.544\times10^{-3}T$
$H°-H°_{298} = 52.826\times10^{-3}T + 1.772\times10^{-6}T^{2} - 16.665$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -721.196 - 4.238\times10^{-3}T + 2.820\times10^{-6}T^{2} + 151.600T^{-1}$
$\Delta Gf° = -721.196 + 4.238\times10^{-3}T\ln T - 2.820\times10^{-6}T^{2} + 75.800T^{-1} + 104.548\times10^{-3}T$
336.35-933.61 K: $\Delta Hf° = -721.192 - 10.037\times10^{-3}T + 12.772\times10^{-6}T^{2} + 240.200T^{-1}$
$\Delta Gf° = -721.192 + 10.037\times10^{-3}T\ln T - 12.772\times10^{-6}T^{2} + 120.100T^{-1} + 73.755\times10^{-3}T$
933.61-955 K: $\Delta Hf° = -722.460 - 13.035\times10^{-3}T + 14.499\times10^{-6}T^{2} + 222.800T^{-1}$
$\Delta Gf° = -722.460 + 13.035\times10^{-3}T\ln T - 14.499\times10^{-6}T^{2} + 111.400T^{-1} + 56.231\times10^{-3}T$
955-1043.7 K: $\Delta Hf° = -725.793 + 5.343\times10^{-3}T - 0.555\times10^{-6}T^{2} - 244.000T^{-1}$
$\Delta Gf° = -725.793 - 5.343\times10^{-3}T\ln T + 0.555\times10^{-6}T^{2} - 122.000T^{-1} + 171.705\times10^{-3}T$
1043.7-1687 K: $\Delta Hf° = -747.396 + 7.681\times10^{-3}T - 0.561\times10^{-6}T^{2} - 107.000T^{-1}$
$\Delta Gf° = -747.396 - 7.681\times10^{-3}T\ln T + 0.561\times10^{-6}T^{2} - 53.500T^{-1} + 208.584\times10^{-3}T$
1687-1800 K: $\Delta Hf° = -772.254 + 6.839\times10^{-3}T + 0.141\times10^{-6}T^{2} + 90.000T^{-1}$
$\Delta Gf° = -772.254 - 6.839\times10^{-3}T\ln T - 0.141\times10^{-6}T^{2} + 45.000T^{-1} + 218.213\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Barany (20). Low-temperature heat capacities and entropy at 298 K from Kelley (250). High-temperature data based on Pankratz (382).

$KAlSi_3O_8(c)$
Potassium Aluminum Trisilicate, Microcline

[Formation: $K(c,l,g) + Al(c,l) + 3Si(c) + 4O_2(g) = KAlSi_3O_8(\text{microcline})$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	48.370	51.200	51.200	0	-948.300	-894.468	655.654
300	48.540	51.500	51.200	.090	-948.313	-894.133	651.367
336.35	51.437	57.217	51.547	1.907	-948.539	-887.556	576.699
336.35	51.437	57.217	51.547	1.907	-949.097	-887.556	576.699
400	56.510	66.620	53.220	5.360	-949.316	-875.899	478.563
500	62.160	79.870	57.250	11.310	-949.295	-857.532	374.822
600	66.140	91.580	62.013	17.740	-948.978	-839.206	305.677
700	69.010	102.000	66.986	24.510	-948.491	-820.941	256.306
800	71.140	111.360	71.960	31.520	-947.919	-802.760	219.301
900	72.800	119.840	76.818	38.720	-947.307	-784.652	190.537
933.61	73.257	122.518	78.415	41.174	-947.096	-778.581	182.257
933.61	73.257	122.518	78.415	41.174	-949.676	-778.581	182.257
1000	74.160	127.580	81.510	46.070	-949.220	-766.404	167.495
1043.7	74.680	130.763	83.506	49.322	-948.911	-758.421	158.811
1043.7	74.680	130.763	83.506	49.322	-967.949	-758.421	158.811
1100	75.350	134.710	86.037	53.540	-967.413	-747.167	148.446
1200	76.470	141.310	90.360	61.140	-966.393	-727.173	132.435
1300	77.590	147.480	94.526	68.840	-965.322	-707.293	118.905
1400	78.750	153.270	98.520	76.650	-964.195	-687.477	107.319

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 61.941 + 13.528\text{x}10^{-3}T - 15.649\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 61.941\text{x}10^{-3}T + 6.764\text{x}10^{-6}T^{2} + 15.649\text{x}10^{2}T^{-1} - 24.318$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -954.375 + 10.346\text{x}10^{-3}T - 8.096\text{x}10^{-6}T^{2} + 1106.000T^{-1}$
$\Delta Gf° = -954.375 - 10.346\text{x}10^{-3}T\ln T + 8.096\text{x}10^{-6}T^{2} + 553.000T^{-1} + 251.240\text{x}10^{-3}T$
336.35-933.61 K: $\Delta Hf° = -954.371 + 4.547\text{x}10^{-3}T + 1.856\text{x}10^{-6}T^{2} + 1194.600T^{-1}$
$\Delta Gf° = -954.371 - 4.547\text{x}10^{-3}T\ln T - 1.856\text{x}10^{-6}T^{2} + 597.300T^{-1} + 220.446\text{x}10^{-3}T$
933.61-1043.7 K: $\Delta Hf° = -955.639 + 1.549\text{x}10^{-3}T + 3.583\text{x}10^{-6}T^{2} + 1177.200T^{-1}$
$\Delta Gf° = -955.639 - 1.549\text{x}10^{-3}T\ln T - 3.583\text{x}10^{-6}T^{2} + 588.600T^{-1} + 202.923\text{x}10^{-3}T$
1043.7-1400 K: $\Delta Hf° = -977.242 + 3.887\text{x}10^{-3}T + 3.577\text{x}10^{-6}T^{2} + 1314.200T^{-1}$
$\Delta Gf° = -977.242 - 3.887\text{x}10^{-3}T\ln T - 3.577\text{x}10^{-6}T^{2} + 657.100T^{-1} + 239.802\text{x}10^{-3}T$

Source: Data from Schumm (438).

$KAlSi_3O_8(c)$
Potassium Aluminum Trisilicate, Sanidine
[Formation: $K(c,l,g) + Al(c,l) + 3Si(c) + 4O_2(g) = KAlSi_3O_8(sanidine)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	48.880	55.670	55.670	0	-946.400	-893.901	655.239
300	49.050	55.970	55.670	.090	-946.413	-893.574	650.960
336.35	51.980	61.747	56.021	1.926	-946.620	-887.160	576.442
336.35	51.980	61.747	56.021	1.926	-947.178	-887.160	576.442
400	57.110	71.260	57.710	5.420	-947.356	-875.795	478.506
500	62.680	84.640	61.780	11.430	-947.275	-857.897	374.982
600	66.590	96.430	66.597	17.900	-946.918	-840.056	305.986
700	69.420	106.920	71.620	24.710	-946.391	-822.285	256.726
800	71.520	116.330	76.630	31.760	-945.779	-804.596	219.803
900	73.160	124.850	81.517	39.000	-945.127	-786.981	191.103
933.61	73.607	127.541	83.125	41.466	-944.904	-781.079	182.841
933.61	73.607	127.541	83.125	41.466	-947.484	-781.079	182.841
1000	74.490	132.630	86.250	46.380	-947.010	-769.244	168.116
1043.7	74.993	135.827	88.259	49.646	-946.687	-761.482	159.452
1043.7	74.993	135.827	88.259	49.646	-965.725	-761.482	159.452
1100	75.640	139.790	90.799	53.890	-965.163	-750.505	149.110
1200	76.680	146.410	95.152	61.510	-964.123	-731.023	133.136
1300	77.670	152.590	99.336	69.230	-963.032	-711.646	119.637
1400	78.680	158.380	103.351	77.040	-961.905	-692.341	108.078
1423	78.920	159.670	104.252	78.860	-961.628	-687.915	105.651

Phase changes:
336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1423 K, incongruent melting point of $KAlSi_3O_8$ to $KAlSi_2O_6$ and liquid.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1423 K:
$Cp° = 63.077 + 12.558x10^{-3}T - 15.949x10^{5}T^{-2}$
$H°- H°_{298} = 63.077x10^{-3}T + 6.279x10^{-6}T^{2} + 15.949x10^{2}T^{-1} - 24.714$

Formation equations (kcal/mol):

298.15-336.35 K:
$ΔHf° = -952.871 + 11.482x10^{-3}T - 8.581x10^{-6}T^{2} + 1136.000T^{-1}$
$ΔGf° = -952.871 - 11.482x10^{-3}TlnT + 8.581x10^{-6}T^{2} + 568.000T^{-1} + 254.258x10^{-3}T$

336.35-933.61 K:
$ΔHf° = -952.867 + 5.683x10^{-3}T + 1.371x10^{-6}T^{2} + 1224.600T^{-1}$
$ΔGf° = -952.867 - 5.683x10^{-3}TlnT - 1.371x10^{-6}T^{2} + 612.300T^{-1} + 223.464x10^{-3}T$

933.61-1043.7 K:
$ΔHf° = -954.135 + 2.685x10^{-3}T + 3.098x10^{-6}T^{2} + 1207.200T^{-1}$
$ΔGf° = -954.135 - 2.685x10^{-3}TlnT - 3.098x10^{-6}T^{2} + 603.600T^{-1} + 205.941x10^{-3}T$

1043.7-1423 K:
$ΔHf° = -975.738 + 5.023x10^{-3}T + 3.092x10^{-6}T^{2} + 1344.200T^{-1}$
$ΔGf° = -975.738 - 5.023x10^{-3}TlnT - 3.092x10^{-6}T^{2} + 672.100T^{-1} + 242.820x10^{-3}T$

Source: Data from Schumm (438).

$KAlSi_3O_8$(vitreous)
Potassium Aluminum Trisilicate
[Formation: $K(c,l,g) + Al(c,l) + 3Si(c) + 4O_2(g) = KAlSi_3O_8(vit)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	50.050	62.520	62.520	0	-935.700	-885.243	648.892
300	50.230	62.830	62.530	.090	-935.713	-884.932	644.664
336.35	53.200	68.745	62.888	1.970	-935.876	-878.770	570.990
336.35	53.200	68.745	62.888	1.970	-936.434	-878.770	570.990
400	58.400	78.470	64.595	5.550	-936.526	-867.849	474.165
500	63.970	92.140	68.760	11.690	-936.315	-850.687	371.830
600	67.870	104.170	73.687	18.290	-935.828	-833.610	303.638
700	70.660	114.860	78.831	25.220	-935.181	-816.633	254.961
800	72.680	124.430	83.930	32.400	-934.439	-799.736	218.475
900	74.160	133.080	88.924	39.740	-933.687	-782.948	190.123
933.61	74.530	135.806	90.563	42.239	-933.432	-777.323	181.962
933.61	74.530	135.806	90.563	42.239	-936.012	-777.323	181.962
1000	75.260	140.950	93.730	47.220	-935.470	-766.024	167.412
1043.7	75.614	144.177	95.775	50.517	-935.117	-758.626	158.854
1043.7	75.614	144.177	95.775	50.517	-954.155	-758.626	158.854
1100	76.070	148.170	98.370	54.780	-953.573	-748.133	148.638
1200	76.670	154.810	102.793	62.420	-952.513	-729.493	132.857
1300	77.120	160.970	107.039	70.110	-951.452	-710.960	119.522

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 63.481 + 13.436\times10^{-3}T - 15.500\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 63.481\times10^{-3}T + 6.718\times10^{-6}T^{2} + 15.500\times10^{2}T^{-1} - 24.723$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -942.180 + 11.886\times10^{-3}T - 8.142\times10^{-6}T^{2} + 1091.100T^{-1}$
$\Delta Gf^\circ = -942.180 - 11.886\times10^{-3}T\ln T + 8.142\times10^{-6}T^{2} + 545.550T^{-1} + 250.123\times10^{-3}T$
336.35-933.61 K: $\Delta Hf^\circ = -942.176 + 6.087\times10^{-3}T + 1.810\times10^{-6}T^{2} + 1179.700T^{-1}$
$\Delta Gf^\circ = -942.176 - 6.087\times10^{-3}T\ln T - 1.810\times10^{-6}T^{2} + 589.850T^{-1} + 219.330\times10^{-3}T$
933.61-1043.7 K: $\Delta Hf^\circ = -943.444 + 3.089\times10^{-3}T + 3.537\times10^{-6}T^{2} + 1162.300T^{-1}$
$\Delta Gf^\circ = -943.444 - 3.089\times10^{-3}T\ln T - 3.537\times10^{-6}T^{2} + 581.150T^{-1} + 201.806\times10^{-3}T$
1043.7-1300 K: $\Delta Hf^\circ = -965.047 + 5.427\times10^{-3}T + 3.531\times10^{-6}T^{2} + 1299.300T^{-1}$
$\Delta Gf^\circ = -965.047 - 5.427\times10^{-3}T\ln T - 3.531\times10^{-6}T^{2} + 649.650T^{-1} + 238.686\times10^{-3}T$

Source: Data from Schumm (438).

KBF_4(c,l)
Potassium Tetrafluoroborate
[Formation: K(c,l) + B(β) + $2F_2$(g) = KBF_4(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	27.500	37.560	37.560	0	-449.800	-427.083	313.056
300	27.560	37.730	37.563	.050	-449.796	-426.942	311.023
336.35	28.898	40.959	37.759	1.076	-449.694	-424.179	275.615
336.35	28.898	40.959	37.759	1.076	-450.252	-424.179	275.615
400	31.240	46.160	38.685	2.990	-450.025	-419.264	229.072
500	35.090	53.540	40.940	6.300	-449.473	-411.635	179.923
556	37.270	57.380	42.395	8.330	-449.037	-407.418	160.144
556	34.950	63.310	42.395	11.630	-445.737	-407.418	160.144
600	34.950	65.970	44.020	13.170	-445.464	-404.391	147.297
700	34.950	71.360	47.560	16.660	-444.904	-397.596	124.133
800	34.950	76.030	50.830	20.160	-444.386	-390.872	106.780
843	34.950	77.860	52.166	21.660	-444.181	-388.004	100.590
843	40.000	82.960	52.166	25.960	-439.881	-388.004	100.590
900	40.000	85.580	54.202	28.240	-439.329	-384.514	93.371

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
556 K, α - β transition point of KBF_4; ΔH° = 3.300 kcal/mol.
843 K, melting point of KBF_4; ΔH° = 4.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-556 K: $Cp^\circ = 15.188 + 39.354\text{x}10^{-3}T + 0.514\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 15.188\text{x}10^{-3}T + 19.677\text{x}10^{-6}T^2 - 0.514\text{x}10^{2}T^{-1} - 6.105$
556-843 K: $Cp^\circ = 34.948$
$H^\circ - H^\circ_{298} = 34.948\text{x}10^{-3}T - 7.801$
843-900 K: $Cp^\circ = 40.000$
$H^\circ - H^\circ_{298} = 40.000\text{x}10^{-3}T - 7.760$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -446.707 - 7.597\text{x}10^{-3}T + 8.569\text{x}10^{-6}T^2 - 473.900T^{-1}$
$\Delta Gf^\circ = -446.707 + 7.597\text{x}10^{-3}T\ln T - 8.569\text{x}10^{-6}T^2 - 236.950T^{-1} + 27.755\text{x}10^{-3}T$
336.35-556 K: $\Delta Hf^\circ = -446.704 - 13.396\text{x}10^{-3}T + 18.521\text{x}10^{-6}T^2 - 385.300T^{-1}$
$\Delta Gf^\circ = -446.704 + 13.396\text{x}10^{-3}T\ln T - 18.521\text{x}10^{-6}T^2 - 192.650T^{-1} - 3.038\text{x}10^{-3}T$
556-843 K: $\Delta Hf^\circ = -448.400 + 6.364\text{x}10^{-3}T - 1.156\text{x}10^{-6}T^2 - 333.900T^{-1}$
$\Delta Gf^\circ = -448.400 - 6.364\text{x}10^{-3}T\ln T + 1.156\text{x}10^{-6}T^2 - 166.950T^{-1} + 113.888\text{x}10^{-3}T$
843-900 K: $\Delta Hf^\circ = -448.359 + 11.416\text{x}10^{-3}T - 1.156\text{x}10^{-6}T^2 - 333.900T^{-1}$
$\Delta Gf^\circ = -448.359 - 11.416\text{x}10^{-3}T\ln T + 1.156\text{x}10^{-6}T^2 - 166.950T^{-1} + 147.874\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Callanan (64). High-temperature data based on Dworkin (133).

$KBH_4(c)$
Potassium Borohydride
[Formation: $K(c,l) + B(\beta) + 2H_2(g) = KBH_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	22.958	25.404	25.404	0	-54.350	-38.287	28.064
300	23.016	25.547	25.404	.043	-54.351	-38.186	27.818
336.35	23.419	28.202	25.565	.887	-54.384	-36.225	23.538
336.35	23.419	28.202	25.565	.887	-54.942	-36.225	23.538
400	24.125	32.385	26.330	2.422	-54.991	-32.683	17.857
500	24.403	37.794	28.102	4.846	-55.115	-27.091	11.841
600	25.339	42.311	30.103	7.325	-55.237	-21.476	7.823
700	27.531	46.362	32.138	9.957	-55.243	-15.843	4.946

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 22.438 + 5.694\times10^{-3}T - 1.046\times10^{5}T^{-2}$

$H°-H°_{298} = 22.438\times10^{-3}T + 2.847\times10^{-6}T^{2} + 1.046\times10^{2}T^{-1} - 7.294$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -54.411 + 3.757\times10^{-3}T - 8.751\times10^{-6}T^{2} - 83.900T^{-1}$

$\Delta Gf° = -54.411 - 3.757\times10^{-3}T\ln T + 8.751\times10^{-6}T^{2} - 41.950T^{-1} + 73.350\times10^{-3}T$

336.35-700 K: $\Delta Hf° = -54.408 - 2.042\times10^{-3}T + 1.201\times10^{-6}T^{2} + 4.700T^{-1}$

$\Delta Gf° = -54.408 + 2.042\times10^{-3}T\ln T - 1.201\times10^{-6}T^{2} + 2.350T^{-1} + 42.557\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from Furukawa (166).

$KBO_2(c,l,g)$
Potassium Borate
[Formation: $K(c,l,g) + B(\beta) + O_2(g) = KBO_2(c,l,g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	16.020	19.116	19.116	0	-237.800	-223.860	164.091
300*	16.070	19.215	19.116	.030	-237.801	-223.772	163.015
336.35	16.888	21.100	19.230	.629	-237.833	-222.070	144.292
336.35	16.888	21.100	19.230	.629	-238.391	-222.070	144.292
400	18.320	24.158	19.776	1.753	-238.419	-218.981	119.644
500	20.070	28.441	21.089	3.676	-238.377	-214.122	93.591
600	21.470	32.228	22.636	5.755	-238.254	-209.284	76.231
700	22.600	35.625	24.254	7.960	-238.061	-204.468	63.837
800	23.540	38.706	25.871	10.268	-237.809	-199.687	54.551
900	24.320	41.525	27.455	12.663	-237.509	-194.937	47.337
1000	24.970	44.122	28.994	15.128	-237.180	-190.225	41.573
1043.7	25.184	45.195	29.650	16.224	-237.030	-188.175	39.403
1043.7	25.184	45.195	29.650	16.224	-256.068	-188.175	39.403
1100	25.460	46.526	30.480	17.651	-255.737	-184.527	36.662
1200	25.780	48.757	31.910	20.216	-255.136	-178.077	32.432
1220	25.810	49.286	32.293	20.732	-255.016	-176.919	31.693
1220	35.000	55.434	32.293	28.232	-247.516	-176.919	31.693
1300	35.000	57.657	33.786	31.032	-246.306	-172.326	28.970
1400	35.000	60.251	35.585	34.532	-244.815	-166.691	26.021
1500	35.000	62.665	37.310	38.032	-243.345	-161.157	23.480
1600	35.000	64.924	38.967	41.532	-241.898	-155.738	21.273
1674.6	35.000	66.519	40.159	44.143	-240.830	-151.745	19.804
1674.6	19.236	100.617	40.159	101.243	-183.730	-151.745	19.804
1700	19.254	100.909	41.064	101.737	-183.764	-151.258	19.445
1800	19.316	102.011	44.421	103.662	-183.932	-149.332	18.131
1900	19.368	103.057	47.480	105.596	-184.111	-147.405	16.955
2000	19.414	104.051	50.283	107.536	-184.305	-145.479	15.897

*Data estimated 310-1674.6 K except temperature and enthalpy of fusion.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1220 K, melting point of KBO_2; ΔH° = 7.500 kcal/mol.
1674.6 K, boiling point of KBO_2; ΔH° = 57.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1220 K: $Cp^\circ = 18.165 + 7.066\text{x}10^{-3}T - 3.780\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 18.165\text{x}10^{-3}T + 3.533\text{x}10^{-6}T^2 + 3.780\text{x}10^{2}T^{-1} - 6.998$
1220-1674.6 K: $Cp^\circ = 35.000$
$H^\circ - H^\circ_{298} = 35.000\text{x}10^{-3}T - 14.468$
1674.6-2000 K: $Cp^\circ = 23.728 - 1.442\text{x}10^{-3}T - 58.243\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 23.728\text{x}10^{-3}T - 0.721\text{x}10^{-6}T^2 + 58.243\text{x}10^{2}T^{-1} + 60.052$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -239.026 + 5.166\text{x}10^{-3}T - 7.730\text{x}10^{-6}T^2 + 111.300T^{-1}$
$\Delta Gf^\circ = -239.026 - 5.166\text{x}10^{-3}T\ln T + 7.730\text{x}10^{-6}T^2 + 55.650T^{-1} + 77.372\text{x}10^{-3}T$
336.35-1043.7 K: $\Delta Hf^\circ = -239.023 - 0.633\text{x}10^{-3}T + 2.222\text{x}10^{-6}T^2 + 199.900T^{-1}$
$\Delta Gf^\circ = -239.023 + 0.633\text{x}10^{-3}T\ln T - 2.222\text{x}10^{-6}T^2 + 99.950T^{-1} + 46.579\text{x}10^{-3}T$
1043.7-1220 K: $\Delta Hf^\circ = -260.626 + 1.705\text{x}10^{-3}T + 2.216\text{x}10^{-6}T^2 + 336.900T^{-1}$
$\Delta Gf^\circ = -260.626 - 1.705\text{x}10^{-3}T\ln T - 2.216\text{x}10^{-6}T^2 + 168.450T^{-1} + 83.459\text{x}10^{-3}T$
1220-1674.6 K: $\Delta Hf^\circ = -268.096 + 18.540\text{x}10^{-3}T - 1.317\text{x}10^{-6}T^2 - 41.100T^{-1}$
$\Delta Gf^\circ = -268.096 - 18.540\text{x}10^{-3}T\ln T + 1.317\text{x}10^{-6}T^2 - 20.550T^{-1} + 205.038\text{x}10^{-3}T$
1674.6-2000 K: $\Delta Hf^\circ = -193.576 + 7.268\text{x}10^{-3}T - 2.038\text{x}10^{-6}T^2 + 5783.200T^{-1}$
$\Delta Gf^\circ = -193.576 - 7.268\text{x}10^{-3}T\ln T + 2.038\text{x}10^{-6}T^2 + 2891.600T^{-1} + 74.617\text{x}10^{-3}T$

Source: Data from Chase (81) who estimated heat capacities 310-1674.6 K.

$KBO_2(g)$
Potassium Borate (ideal gas)
[Formation: $K(c,l,g) + B(\beta) + O_2(g) = KBO_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	14.106	71.055	71.055	0	-161.100	-162.645	119.221
300	14.133	71.143	71.056	.026	-161.105	-162.654	118.492
336.35	14.555	72.784	71.156	.547	-161.214	-162.835	105.804
336.35	14.555	72.784	71.156	.547	-161.772	-162.835	105.804
400	15.294	75.377	71.624	1.501	-161.971	-163.021	89.069
500	16.157	78.886	72.736	3.075	-162.278	-163.246	71.354
600	16.822	81.893	74.018	4.725	-162.584	-163.413	59.522
700	17.344	84.527	75.334	6.435	-162.886	-163.524	51.054
800	17.757	86.871	76.632	8.191	-163.186	-163.596	44.692
900	18.086	88.983	77.891	9.983	-163.489	-163.629	39.734
1000	18.350	90.902	79.096	11.806	-163.802	-163.627	35.760
1043.7	18.443	91.689	79.607	12.610	-163.944	-163.615	34.260
1043.7	18.443	91.689	79.607	12.610	-182.982	-163.615	34.260
1100	18.563	92.662	80.251	13.652	-183.036	-162.576	32.300
1200	18.737	94.284	81.353	15.517	-183.135	-160.708	29.269
1300	18.880	95.790	82.407	17.398	-183.240	-158.833	26.702
1400	18.999	97.194	83.414	19.292	-183.355	-156.951	24.501
1500	19.099	98.508	84.377	21.197	-183.480	-155.056	22.591
1600	19.183	99.743	85.298	23.112	-183.618	-153.168	20.922
1700	19.254	100.909	86.184	25.033	-183.768	-151.262	19.446
1800	19.316	102.011	87.032	26.962	-183.932	-149.332	18.131
1900	19.368	103.057	87.849	28.896	-184.111	-147.405	16.955
2000	19.414	104.051	88.633	30.836	-184.305	-145.479	15.897

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 16.495 + 1.854\text{x}10^{-3}T - 2.615\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 16.495\text{x}10^{-3}T + 0.927\text{x}10^{-6}T^2 + 2.615\text{x}10^{2}T^{-1} - 5.877$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -161.206 + 3.496\text{x}10^{-3}T - 10.336\text{x}10^{-6}T^2 - 5.200T^{-1}$
$\Delta Gf^\circ = -161.206 - 3.496\text{x}10^{-3}T\ln T + 10.336\text{x}10^{-6}T^2 - 2.600T^{-1} + 12.039\text{x}10^{-3}T$
336.35-1043.7 K: $\Delta Hf^\circ = -161.203 - 2.303\text{x}10^{-3}T - 0.384\text{x}10^{-6}T^2 + 83.400T^{-1}$
$\Delta Gf^\circ = -161.203 + 2.303\text{x}10^{-3}T\ln T + 0.384\text{x}10^{-6}T^2 + 41.700T^{-1} - 18.754\text{x}10^{-3}T$
1043.7-2000 K: $\Delta Hf^\circ = -182.806 + 0.035\text{x}10^{-3}T - 0.390\text{x}10^{-6}T^2 + 220.400T^{-1}$
$\Delta Gf^\circ = -182.806 - 0.035\text{x}10^{-3}T\ln T + 0.390\text{x}10^{-6}T^2 + 110.200T^{-1} + 18.125\text{x}10^{-3}T$

Source: Data from Chase (81) who estimated some molecular constants.

$K_2B_4O_7$(c,l)
Potassium Diborate
[Formation: 2K(c,l,g) + 4B(β) + $3.5O_2$(g) = $K_2B_4O_7$(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	40.750	49.800	49.800	0	-796.900	-749.711	549.546
300	40.950	50.053	49.800	.076	-796.916	-749.413	545.940
336.35	43.985	54.910	50.095	1.620	-797.225	-743.640	483.188
336.35	43.985	54.910	50.095	1.620	-798.341	-743.640	483.188
400	49.300	63.092	51.522	4.628	-798.745	-733.262	400.630
500	55.640	74.813	55.027	9.893	-799.152	-716.827	313.321
600	59.880	85.364	59.221	15.686	-799.354	-700.350	255.099
700	62.710	94.817	63.643	21.822	-799.445	-683.835	213.500
800	64.800	103.334	68.080	28.203	-799.465	-667.317	182.300
900	66.300	111.059	72.433	34.763	-799.454	-650.797	158.033
1000	67.700	118.118	76.654	41.464	-799.441	-634.280	138.620
1043.7	68.226	121.025	78.451	44.434	-799.435	-627.061	131.304
1043.7	68.226	121.025	78.451	44.434	-837.511	-627.061	131.304
1088	68.760	123.874	80.253	47.460	-837.305	-618.166	124.171
1088	109.423	146.815	80.253	72.420	-812.345	-618.166	124.171
1100	109.790	148.018	80.985	73.736	-811.796	-616.027	122.392
1200	112.606	157.693	86.978	84.858	-807.112	-598.426	108.987
1300	115.180	166.810	92.772	96.249	-802.245	-581.219	97.711
1400	117.512	175.433	98.372	107.886	-797.218	-564.405	88.106
1500	119.600	183.613	103.784	119.744	-792.051	-547.940	79.834
1600	121.446	191.392	109.018	131.798	-786.774	-531.887	72.651

*Entropy at 298 K estimated and heat capacities extrapolated above 973 K.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1088 K, melting point of $K_2B_4O_7$; ΔH° = 24.960 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1088 K:
$Cp° = 54.248 + 15.602\times10^{-3}T - 16.134\times10^{5}T^{-2}$
$H°-H°_{298} = 54.248\times10^{-3}T + 7.801\times10^{-6}T^{2} + 16.134\times10^{2}T^{-1} - 22.279$

1088-1600 K:
$Cp° = 100.568 + 15.596\times10^{-3}T - 96.037\times10^{5}T^{-2}$
$H°-H°_{298} = 100.568\times10^{-3}T + 7.798\times10^{-6}T^{2} + 96.037\times10^{2}T^{-1} - 55.056$

Formation equations (kcal/mol):

298.15-336.35 K:
$\Delta Hf° = -799.683 + 7.959\times10^{-3}T - 16.864\times10^{-6}T^{2} + 569.200T^{-1}$
$\Delta Gf° = -799.683 - 7.959\times10^{-3}T\ln T + 16.864\times10^{-6}T^{2} + 284.600T^{-1} + 204.724\times10^{-3}T$

336.35-1043.7 K:
$\Delta Hf° = -799.677 - 3.639\times10^{-3}T + 3.040\times10^{-6}T^{2} + 746.400T^{-1}$
$\Delta Gf° = -799.677 + 3.639\times10^{-3}T\ln T - 3.040\times10^{-6}T^{2} + 373.200T^{-1} + 143.137\times10^{-3}T$

1043.7-1088 K:
$\Delta Hf° = -842.882 + 1.037\times10^{-3}T + 3.029\times10^{-6}T^{2} + 1020.400T^{-1}$
$\Delta Gf° = -842.882 - 1.037\times10^{-3}T\ln T - 3.029\times10^{-6}T^{2} + 510.200T^{-1} + 216.896\times10^{-3}T$

1088-1600 K:
$\Delta Hf° = -875.659 + 47.357\times10^{-3}T + 3.025\times10^{-6}T^{2} + 9010.700T^{-1}$
$\Delta Gf° = -875.659 - 47.357\times10^{-3}T\ln T - 3.025\times10^{-6}T^{2} + 4505.350T^{-1} + 567.518\times10^{-3}T$

Source: Data from JANAF (127) who estimated entropy at 298 K and extrapolated heat capacities above 973 K.

$K_2B_6O_{10}$(c)
Potassium Triborate
[Formation: $2K(c,l,g) + 6B(\beta) + 5O_2(g) = K_2B_6O_{10}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	62.600	60.000	60.000	0	-1113.500	-1046.595	767.165
300	62.700	60.388	60.001	.116	-1113.505	-1046.173	762.127
336.35	64.736	67.675	60.444	2.432	-1113.633	-1038.008	674.457
336.35	64.736	67.675	60.444	2.432	-1114.749	-1038.008	674.457
400	68.300	79.197	62.527	6.668	-1115.033	-1023.474	559.193
500	73.680	95.019	67.483	13.768	-1115.516	-1000.513	437.318
600	78.900	108.916	73.253	21.398	-1115.963	-977.484	356.044
700	84.000	121.461	79.257	29.543	-1116.248	-954.368	297.963
800	89.100	133.013	85.264	38.199	-1116.282	-931.238	254.399
900	94.040	143.795	91.174	47.359	-1116.030	-908.116	220.518
1000	98.670	153.962	96.950	57.012	-1115.482	-885.040	193.423
1043.7	99.762	158.206	99.427	61.348	-1115.182	-874.975	183.217
1043.7	99.762	158.206	99.427	61.348	-1153.258	-874.975	183.217
1100	101.170	163.490	102.570	67.012	-1152.575	-860.015	170.867

*Entropy at 298 K estimated.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 50.528 + 48.154\times10^{-3}T - 2.031\times10^{5}T^{-2}$
$H° - H°_{298} = 50.528\times10^{-3}T + 24.077\times10^{-6}T^{2} + 2.031\times10^{2}T^{-1} - 17.886$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -1103.938 - 16.052\times10^{-3}T - 2.726\times10^{-6}T^{2} - 1351.900T^{-1}$
$\Delta Gf° = -1103.938 + 16.052\times10^{-3}T\ln T + 2.726\times10^{-6}T^{2} - 675.950T^{-1} + 107.660\times10^{-3}T$
336.35-1043.7 K: $\Delta Hf° = -1103.931 - 27.650\times10^{-3}T + 17.178\times10^{-6}T^{2} - 1174.700T^{-1}$
$\Delta Gf° = -1103.931 + 27.650\times10^{-3}T\ln T - 17.178\times10^{-6}T^{2} - 587.350T^{-1} + 46.072\times10^{-3}T$
1043.7-1100 K: $\Delta Hf° = -1147.137 - 22.974\times10^{-3}T + 17.166\times10^{-6}T^{2} - 900.700T^{-1}$
$\Delta Gf° = -1147.137 + 22.974\times10^{-3}T\ln T - 17.166\times10^{-6}T^{2} - 450.350T^{-1} + 119.832\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127) who estimated entropy at 298 K.

$K_2B_8O_{13}$(c,l)
Potassium Tetraborate
[Formation: $2K(c,l,g) + 8B(\beta) + 6.5O_2(g) = K_2B_8O_{13}(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	76.790	70.200	70.200	0	-1428.100	-1341.479	983.318
300	76.970	70.676	70.203	.142	-1428.109	-1340.933	976.857
336.35	80.311	79.670	70.749	3.001	-1428.285	-1330.360	864.416
336.35	80.311	79.670	70.749	3.001	-1429.401	-1330.360	864.416
400	86.160	94.086	73.331	8.302	-1429.727	-1311.606	716.619
500	94.960	114.253	79.541	17.356	-1430.167	-1282.000	560.355
600	104.000	132.371	86.859	27.307	-1430.375	-1252.362	456.167
700	112.680	149.077	94.568	38.156	-1430.159	-1222.690	381.736
800	119.600	164.587	102.365	49.778	-1429.516	-1193.092	325.933
900	125.500	179.023	110.089	62.041	-1428.521	-1163.591	282.555
1000	130.500	192.518	117.665	74.853	-1427.230	-1134.219	247.880
1043.7	132.029	198.132	120.918	80.589	-1426.601	-1121.426	234.823
1043.7	132.029	198.132	120.918	80.589	-1464.677	-1121.426	234.823
1100	134.000	205.122	125.048	88.081	-1463.561	-1102.985	219.140
1130	135.000	208.740	127.227	92.110	-1462.952	-1093.164	211.423
1130	158.100	235.200	127.227	122.010	-1433.052	-1093.164	211.423
1200	158.100	244.702	133.805	133.077	-1430.023	-1072.183	195.269

*Entropy at 298 K estimated.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1130 K, melting point of $K_2B_8O_{13}$; ΔH° = 29.900 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1130 K: $Cp° = 68.503 + 63.014\times10^{-3}T - 9.335\times10^{5}T^{-2}$
$H°- H°_{298} = 68.503\times10^{-3}T + 31.507\times10^{-6}T^{2} + 9.335\times10^{2}T^{-1} - 26.356$
1130-1200 K: $Cp° = 158.100$
$H°- H°_{298} = 158.100\times10^{-3}T - 56.643$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -1419.054 - 18.368\times10^{-3}T + 2.565\times10^{-6}T^{2} - 1132.300T^{-1}$
$\Delta Gf° = -1419.054 + 18.368\times10^{-3}T\ln T - 2.565\times10^{-6}T^{2} - 566.150T^{-1} + 162.666\times10^{-3}T$
336.35-1043.7 K: $\Delta Hf° = -1419.047 - 29.966\times10^{-3}T + 22.469\times10^{-6}T^{2} - 955.100T^{-1}$
$\Delta Gf° = -1419.047 + 29.966\times10^{-3}T\ln T - 22.469\times10^{-6}T^{2} - 477.550T^{-1} + 101.079\times10^{-3}T$
1043.7-1130 K: $\Delta Hf° = -1462.253 - 25.290\times10^{-3}T + 22.458\times10^{-6}T^{2} - 681.100T^{-1}$
$\Delta Gf° = -1462.253 + 25.290\times10^{-3}T\ln T - 22.458\times10^{-6}T^{2} - 340.550T^{-1} + 174.838\times10^{-3}T$
1130-1200 K: $\Delta Hf° = -1492.541 + 64.307\times10^{-3}T - 9.049\times10^{-6}T^{2} - 1614.600T^{-1}$
$\Delta Gf° = -1492.541 - 64.307\times10^{-3}T\ln T + 9.049\times10^{-6}T^{2} - 807.300T^{-1} + 796.268\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127) who estimated entropy at 298 K.

$KCN(c,l)$
Potassium Cyanide
[Formation: $K(c,l,g) + C(c) + 0.5N_2(g) = KCN(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.868	30.540	30.540	0	-27.120	-24.385	17.874
300*	15.866	30.638	30.541	.029	-27.115	-24.368	17.752
336.35	15.860	32.452	30.652	.606	-27.015	-24.041	15.621
336.35	15.860	32.452	30.652	.606	-27.573	-24.041	15.621
400	15.850	35.198	31.163	1.614	-27.436	-23.386	12.777
500	15.859	38.736	32.336	3.200	-27.261	-22.394	9.789
600	15.868	41.628	33.651	4.786	-27.135	-21.433	7.807
700	15.878	44.075	34.971	6.373	-27.052	-20.490	6.397
800	15.887	46.196	36.243	7.962	-27.005	-19.556	5.342
895	15.897	47.979	37.396	9.472	-26.994	-18.673	4.560
895	18.000	51.890	37.396	12.972	-23.494	-18.673	4.560
900	18.000	51.990	37.477	13.062	-23.484	-18.646	4.528
1000	18.000	53.887	39.025	14.862	-23.299	-18.120	3.960
1043.7	18.000	54.657	39.664	15.649	-23.230	-17.894	3.747
1043.7	18.000	54.657	39.664	15.649	-42.268	-17.894	3.747
1100	18.000	55.602	40.455	16.662	-42.054	-16.574	3.293
1200	18.000	57.169	41.784	18.462	-41.689	-14.285	2.602
1300	18.000	58.609	43.023	20.262	-41.341	-12.014	2.020
1400	18.000	59.943	44.184	22.062	-41.007	-9.771	1.525
1500	18.000	61.185	45.277	23.862	-40.687	-7.551	1.100
1600	18.000	62.347	46.308	25.662	-40.376	-5.353	.731
1700	18.000	63.438	47.284	27.462	-40.077	-3.174	.408
1800	18.000	64.467	48.210	29.262	-39.787	-1.011	.123
1900	18.000	65.440	49.092	31.062	-39.505	1.136	-.131
2000	18.000	66.364	49.933	32.862	-39.233	3.267	-.357

*Data above 298 K estimated except temperature and enthalpy of fusion.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
895 K, melting point of KCN; ΔH° = 3.500 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-895 K: $Cp° = 15.723 + 0.198\times10^{-3}T + 0.076\times10^{5}T^{-2}$
$H°- H°_{298} = 15.723\times10^{-3}T + 0.099\times10^{-6}T^{2} - 0.076\times10^{2}T^{-1} - 4.671$
895-2000 K: $Cp° = 18.000$
$H°- H°_{298} = 18.000\times10^{-3}T - 3.138$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -27.905 + 7.900\times10^{-3}T - 11.030\times10^{-6}T^{2} - 175.950T^{-1}$
$\Delta Gf° = -27.905 - 7.900\times10^{-3}T\ln T + 11.030\times10^{-6}T^{2} - 87.975T^{-1} + 54.522\times10^{-3}T$
336.35-895 K: $\Delta Hf° = -27.902 + 2.101\times10^{-3}T - 1.078\times10^{-6}T^{2} - 87.350T^{-1}$
$\Delta Gf° = -27.902 - 2.101\times10^{-3}T\ln T + 1.078\times10^{-6}T^{2} - 43.675T^{-1} + 23.729\times10^{-3}T$
895-1043.7 K: $\Delta Hf° = -26.369 + 4.378\times10^{-3}T - 1.177\times10^{-6}T^{2} - 79.750T^{-1}$
$\Delta Gf° = -26.369 - 4.378\times10^{-3}T\ln T + 1.177\times10^{-6}T^{2} - 39.875T^{-1} + 37.399\times10^{-3}T$
1043.7-2000 K: $\Delta Hf° = -47.972 + 6.716\times10^{-3}T - 1.183\times10^{-6}T^{2} + 57.250T^{-1}$
$\Delta Gf° = -47.972 - 6.716\times10^{-3}T\ln T + 1.183\times10^{-6}T^{2} + 28.625T^{-1} + 74.278\times10^{-3}T$

Source: Data from JANAF (127) who estimated all above 310 K except temperature and enthalpy of fusion.

KCN(g)
Potassium Cyanide (ideal gas)
[Formation: K(c,l,g) + C(c) + 0.5N$_2$(g) = KCN(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°$_{298}$)/T	H°- H°$_{298}$	ΔHf°	ΔGf°	
298.15*	12.155	60.477	60.477	0	22.200	16.010	-11.735
300	12.164	60.552	60.479	.022	22.198	15.971	-11.634
336.35	12.293	61.951	60.564	.467	22.166	15.218	-9.888
336.35	12.293	61.951	60.564	.467	21.608	15.218	-9.888
400	12.520	64.104	60.959	1.258	21.528	14.016	-7.658
500	12.778	66.926	61.880	2.523	21.382	12.154	-5.312
600	13.015	69.277	62.922	3.813	21.212	10.325	-3.761
700	13.238	71.301	63.978	5.126	21.021	8.524	-2.661
800	13.443	73.082	65.007	6.460	20.813	6.753	-1.845
900	13.625	74.676	65.994	7.814	20.589	5.009	-1.216
1000	13.782	76.120	66.936	9.184	20.343	3.289	-.719
1043.7	13.841	76.711	67.333	9.788	20.229	2.547	-.533
1043.7	13.841	76.711	67.333	9.788	1.191	2.547	-.533
1100	13.918	77.440	67.831	10.570	1.174	2.632	-.523
1200	14.034	78.656	68.684	11.967	1.136	2.755	-.502
1300	14.133	79.783	69.494	13.376	1.093	2.893	-.486
1400	14.218	80.834	70.268	14.793	1.044	3.033	-.473
1500	14.290	81.817	71.004	16.219	.991	3.178	-.463
1600	14.352	82.742	71.710	17.651	.933	3.325	-.454
1700	14.406	83.613	72.384	19.089	.870	3.475	-.447
1800	14.453	84.438	73.031	20.532	.803	3.631	-.441
1900	14.494	85.221	73.653	21.979	.733	3.789	-.436
2000	14.529	85.965	74.249	23.431	.657	3.954	-.432

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.500 + 1.228\times10^{-3}T - 0.632\times10^{5}T^{-2}$
$H° - H°_{298} = 12.500\times10^{-3}T + 0.614\times10^{-6}T^{2} + 0.632\times10^{2}T^{-1} - 3.993$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = 22.093 + 4.678\times10^{-3}T - 10.514\times10^{-6}T^{2} - 105.150T^{-1}$
$\Delta Gf° = 22.093 - 4.678\times10^{-3}T\ln T + 10.514\times10^{-6}T^{2} - 52.575T^{-1} + 3.704\times10^{-3}T$
336.35-1043.7 K: $\Delta Hf° = 22.096 - 1.121\times10^{-3}T - 0.562\times10^{-6}T^{2} - 16.550T^{-1}$
$\Delta Gf° = 22.096 + 1.121\times10^{-3}T\ln T + 0.562\times10^{-6}T^{2} - 8.275T^{-1} - 27.089\times10^{-3}T$
1043.7-2000 K: $\Delta Hf° = 0.493 + 1.217\times10^{-3}T - 0.569\times10^{-6}T^{2} + 120.450T^{-1}$
$\Delta Gf° = 0.493 - 1.217\times10^{-3}T\ln T + 0.569\times10^{-6}T^{2} + 60.225T^{-1} + 9.790\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Skudlarski (464). Other data are those estimated by JANAF (127).

K_2CO_3(c,l)
Potassium Carbonate

[Formation: $2K(c,l,g) + C(c) + 1.5O_2(g) = K_2CO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	27.351	37.170	37.170	0	-274.900	-254.440	186.507
300	27.414	37.339	37.170	.051	-274.898	-254.312	185.264
336.35	28.581	40.541	37.364	1.069	-274.887	-251.819	163.622
336.35	28.581	40.541	37.364	1.069	-276.003	-251.819	163.622
400	30.625	45.675	38.285	2.956	-275.931	-247.248	135.088
500	33.473	52.821	40.493	6.164	-275.622	-240.108	104.950
600	36.010	59.152	43.085	9.640	-275.107	-233.049	84.887
700	38.356	64.881	45.797	13.359	-274.411	-226.093	70.588
800	40.641	70.152	48.516	17.309	-273.542	-219.250	59.895
900	42.905	75.070	51.196	21.487	-272.495	-212.524	51.607
1000	45.160	79.707	53.817	25.890	-271.282	-205.925	45.004
1043.7	46.139	81.660	54.942	27.885	-270.700	-203.080	42.524
1043.7	46.139	81.660	54.942	27.885	-308.776	-203.080	42.524
1100	47.400	84.117	56.373	30.518	-307.710	-197.396	39.218
1174	48.936	87.252	58.221	34.082	-306.219	-190.032	35.376
1174	50.000	92.874	58.221	40.682	-299.619	-190.032	35.376
1200	50.000	93.972	58.987	41.982	-299.051	-187.615	34.169
1300	50.000	97.974	61.834	46.982	-296.876	-178.417	29.994
1400	50.000	101.679	64.549	51.982	-294.725	-169.384	26.442
1500	50.000	105.129	67.141	56.982	-292.592	-160.506	23.385
1600	50.000	108.356	69.617	61.982	-290.478	-151.770	20.731
1700	50.000	111.387	71.986	66.982	-288.377	-143.166	18.405
1800	50.000	114.245	74.255	71.982	-286.294	-134.684	16.353
1900	50.000	116.948	76.431	76.982	-284.225	-126.317	14.530
2000	50.000	119.513	78.522	81.982	-282.173	-118.059	12.901

<ins>Phase changes</ins>: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1174 K, melting point of K_2CO_3; ΔH° = 6.600 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1174 K: $Cp° = 23.361 + 22.016\times10^{-3}T - 2.289\times10^{5}T^{-2}$
$H°-H°_{298} = 23.361\times10^{-3}T + 11.008\times10^{-6}T^{2} + 2.289\times10^{2}T^{-1} - 8.711$
1174-2000 K: $Cp° = 50.000$
$H°-H°_{298} = 50.000\times10^{-3}T - 18.018$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -275.975 + 6.906\times10^{-3}T - 10.649\times10^{-6}T^{2} - 11.200T^{-1}$
$\Delta Gf° = -275.975 - 6.906\times10^{-3}T\ln T + 10.649\times10^{-6}T^{2} - 5.600T^{-1} + 108.464\times10^{-3}T$
336.35-1043.7 K: $\Delta Hf° = -275.968 - 4.692\times10^{-3}T + 9.255\times10^{-6}T^{2} + 166.000T^{-1}$
$\Delta Gf° = -275.968 + 4.692\times10^{-3}T\ln T - 9.255\times10^{-6}T^{2} + 83.000T^{-1} + 46.878\times10^{-3}T$
1043.7-1174 K: $\Delta Hf° = -319.174 - 0.016\times10^{-3}T + 9.244\times10^{-6}T^{2} + 440.000T^{-1}$
$\Delta Gf° = -319.174 + 0.016\times10^{-3}T\ln T - 9.244\times10^{-6}T^{2} + 220.000T^{-1} + 120.637\times10^{-3}T$
1174-2000 K: $\Delta Hf° = -328.481 + 26.623\times10^{-3}T - 1.765\times10^{-6}T^{2} + 211.100T^{-1}$
$\Delta Gf° = -328.481 - 26.623\times10^{-3}T\ln T + 1.765\times10^{-6}T^{2} + 105.550T^{-1} + 304.013\times10^{-3}T$

Source: Data from Chang (74).

$KClO_4(c)$
Potassium Perchlorate
[Formation: $K(c,l) + 0.5Cl_2(g) + 2O_2(g) = KClO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	25.813	35.870	35.870	0	-103.430	-72.350	53.033
300	25.897	36.030	35.870	.048	-103.429	-72.157	52.566
336.35	27.570	39.087	36.053	1.020	-103.389	-68.369	44.424
336.35	27.570	39.087	36.053	1.020	-103.947	-68.369	44.424
350	28.198	40.196	36.193	1.401	-103.920	-66.927	41.790
400	30.540	44.114	36.941	2.869	-103.757	-61.652	33.685
450	32.959	47.849	37.947	4.456	-103.480	-56.404	27.393
500	35.452	51.450	39.118	6.166	-103.091	-51.193	22.376
550	38.009	54.949	40.400	8.002	-102.585	-46.026	18.289
573	39.204	56.530	41.015	8.890	-102.312	-43.667	16.655
573	34.310	62.464	41.015	12.290	-98.912	-43.667	16.655
600	34.636	64.051	42.016	13.221	-98.706	-41.068	14.959
650	35.605	66.858	43.820	14.975	-98.303	-36.280	12.198
700	37.050	69.547	45.563	16.789	-97.850	-31.527	9.843
750	38.970	72.166	47.249	18.688	-97.322	-26.810	7.812
800	41.365	74.755	48.887	20.694	-96.696	-22.129	6.045

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
573 K, α - β transition point of $KClO_4$; ΔH° = 3.400 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-573 K: $Cp° = 9.158 + 51.780\times10^{-3}T + 1.082\times10^{5}T^{-2}$
$H° - H°_{298} = 9.158\times10^{-3}T + 25.890\times10^{-6}T^2 - 1.082\times10^{2}T^{-1} - 4.669$
573-800 K: $Cp° = -22.511 + 68.222\times10^{-3}T + 58.215\times10^{5}T^{-2}$
$H° - H°_{298} = -22.511\times10^{-3}T + 34.111\times10^{-6}T^2 - 58.215\times10^{2}T^{-1} + 24.149$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -100.754 - 10.761\times10^{-3}T + 14.772\times10^{-6}T^2 - 232.750T^{-1}$
$\Delta Gf° = -100.754 + 10.761\times10^{-3}T\ln T - 14.772\times10^{-6}T^2 - 116.375T^{-1} + 39.665\times10^{-3}T$
336.35-573 K: $\Delta Hf° = -100.751 - 16.561\times10^{-3}T + 24.724\times10^{-6}T^2 - 144.150T^{-1}$
$\Delta Gf° = -100.751 + 16.561\times10^{-3}T\ln T - 24.724\times10^{-6}T^2 - 72.075T^{-1} + 8.872\times10^{-3}T$
573-800 K: $\Delta Hf° = -71.933 - 48.229\times10^{-3}T + 32.945\times10^{-6}T^2 - 5857.450T^{-1}$
$\Delta Gf° = -71.933 + 48.229\times10^{-3}T\ln T - 32.945\times10^{-6}T^2 - 2928.725T^{-1} - 229.136\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Zalukaev (538). High-temperature data based on Rajeshwar (412).

$K_2Cr_2O_7$(c,l)
Potassium Dichromate
[Formation: $2K(c,l) + 2Cr(c) + 3.5O_2(g) = K_2Cr_2O_7(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	52.400	69.600	69.600	0	-492.700	-449.727	329.655
300	52.540	69.900	69.600	.100	-492.691	-449.451	327.421
311.5	53.642	71.897	69.616	.711	-492.663	-447.794	314.170
336.35	56.022	76.145	70.121	2.026	-492.706	-444.275	288.672
336.35	56.022	76.145	70.121	2.026	-493.822	-444.275	288.672
350	57.330	78.400	70.400	2.800	-493.787	-442.266	276.160
400	62.980	86.400	71.900	5.800	-493.267	-434.955	237.645
450	69.670	94.200	73.756	9.200	-492.495	-427.615	207.675
500	77.500	101.900	76.300	12.800	-491.555	-420.513	183.804
540	84.630	108.100	78.357	16.100	-490.405	-414.833	167.890
540	64.000	108.800	78.357	16.400	-490.105	-414.833	167.890
550	64.300	110.000	78.909	17.100	-489.945	-413.432	164.280
600	65.800	115.600	81.767	20.300	-489.466	-406.516	148.071
650	67.400	121.000	84.692	23.600	-488.916	-399.700	134.390
670	68.000	123.000	85.697	25.000	-488.624	-396.885	129.460
670	98.000	137.200	85.697	34.500	-479.124	-396.885	129.460
700	98.000	141.500	88.071	37.400	-477.895	-393.283	122.787
750	98.000	148.200	91.800	42.300	-475.804	-387.272	112.849
800	98.000	154.600	95.600	47.200	-473.736	-381.497	104.219

Phase changes: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
540 K, α - β transition point of $K_2Cr_2O_7$; ΔH° = 0.300 kcal/mol.
670 K, melting point pf $K_2Cr_2O_7$; ΔH° = 9.500 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-540 K: $Cp° = -27.833 + 196.906x10^{-3}T + 19.137x10^{5}T^{-2}$
$H°- H°_{298} = -27.833x10^{-3}T + 98.453x10^{-6}T^{2} - 19.137x10^{2}T^{-1} + 5.965$
540-670 K: $Cp° = 47.586 + 31.446x10^{-3}T - 1.651x10^{5}T^{-2}$
$H°- H°_{298} = 47.586x10^{-3}T + 15.723x10^{-6}T^{2} + 1.651x10^{2}T^{-1} - 14.187$
670-800 K: $Cp° = 98.000$
$H°- H°_{298} = 98.000x10^{-3}T - 31.160$

Formation equations (kcal/mol):

298.15-311.5 K: $ΔHf° = -475.263 - 49.614x10^{-3}T + 48.422x10^{-6}T^{2} - 2071.900T^{-1}$
$ΔGf° = -475.263 + 49.614x10^{-3}T\ln T - 48.422x10^{-6}T^{2} - 1035.950T^{-1} - 170.943x10^{-3}T$
311.5-336.35 K: $ΔHf° = -473.267 - 63.948x10^{-3}T + 72.975x10^{-6}T^{2} - 2044.700T^{-1}$
$ΔGf° = -473.267 + 63.948x10^{-3}T\ln T - 72.975x10^{-6}T^{2} - 1022.350T^{-1} - 252.138x10^{-3}T$
336.35-540 K: $ΔHf° = -473.261 - 75.546x10^{-3}T + 92.879x10^{-6}T^{2} - 1867.500T^{-1}$
$ΔGf° = -473.261 + 75.546x10^{-3}T\ln T - 92.879x10^{-6}T^{2} - 933.750T^{-1} - 313.724x10^{-3}T$
540-670 K: $ΔHf° = -493.413 - 0.127x10^{-3}T + 10.148x10^{-6}T^{2} + 211.300T^{-1}$
$ΔGf° = -493.413 + 0.127x10^{-3}T\ln T - 10.148x10^{-6}T^{2} + 105.650T^{-1} + 149.859x10^{-3}T$
670-800 K: $ΔHf° = -510.386 + 50.287x10^{-3}T - 5.575x10^{-6}T^{2} + 46.200T^{-1}$
$ΔGf° = -510.386 - 50.287x10^{-3}T\ln T + 5.575x10^{-6}T^{2} + 23.100T^{-1} + 492.899x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Popov (406). High-temperature data based on Holm (207, 208), Kelley (243), Nguyen-Duy (354), and Popov (405).

KH(c)
Potassium Hydride
[Formation: K(c,l) + $0.5H_2(g)$ = KH(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	9.060	12.000	12.000	0	-13.800	-8.117	5.950
300	9.100	12.056	12.000	.017	-13.802	-8.081	5.887
336.35	9.627	13.127	12.064	.357	-13.859	-7.385	4.799
336.35	9.627	13.127	12.064	.357	-14.417	-7.385	4.799
400	10.550	14.906	12.378	1.011	-14.470	-6.050	3.305
500	11.600	17.378	13.138	2.120	-14.453	-3.945	1.725
600	12.410	19.568	14.030	3.323	-14.326	-1.853	.675
700	13.051	21.530	14.963	4.597	-14.119	.211	-.066
800	13.580	23.309	15.898	5.929	-13.852	2.239	-.612

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 9.842 + 5.170\times10^{-3}T - 2.065\times10^{5}T^{-2}$

$H°-H°_{298} = 9.842\times10^{-3}T + 2.585\times10^{-6}T^{2} + 2.065\times10^{2}T^{-1} - 3.857$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -15.497 + 5.568\times10^{-3}T - 7.693\times10^{-6}T^{2} + 214.750T^{-1}$

$\Delta Gf° = -15.497 - 5.568\times10^{-3}T\ln T + 7.693\times10^{-6}T^{2} + 107.375T^{-1} + 52.974\times10^{-3}T$

336.35-800 K: $\Delta Hf° = -15.493 - 0.231\times10^{-3}T + 2.260\times10^{-6}T^{2} + 303.350T^{-1}$

$\Delta Gf° = -15.493 + 0.231\times10^{-3}T\ln T - 2.260\times10^{-6}T^{2} + 151.675T^{-1} + 22.180\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data are those estimated by JANAF (127).

KH(g)
Potassium Hydride (ideal gas)
[Formation: K(c,l,g) + $0.5H_2$(g) = KH(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.418	47.304	47.304	0	31.400	26.557	-19.467
300	7.426	47.350	47.304	.014	31.394	26.527	-19.325
336.35	7.568	48.207	47.356	.287	31.270	25.945	-16.858
336.35	7.568	48.207	47.356	.287	30.712	25.945	-16.858
400	7.818	49.541	47.601	.776	30.495	25.061	-13.693
500	8.134	51.321	48.171	1.575	30.202	23.738	-10.376
600	8.370	52.826	48.824	2.401	29.952	22.470	-8.185
700	8.545	54.130	49.491	3.247	29.731	21.241	-6.632
800	8.678	55.280	50.145	4.108	29.527	20.041	-5.475
900	8.782	56.308	50.774	4.981	29.333	18.867	-4.582
1000	8.867	57.238	51.374	5.864	29.135	17.715	-3.871
1043.7	8.898	57.618	51.628	6.252	29.046	17.218	-3.605
1043.7	8.898	57.618	51.628	6.252	10.008	17.218	-3.605
1100	8.937	58.087	51.947	6.754	10.025	17.606	-3.498
1200	8.996	58.867	52.491	7.651	10.057	18.295	-3.332
1300	9.048	59.589	53.010	8.553	10.090	18.980	-3.191
1400	9.095	60.261	53.504	9.460	10.122	19.663	-3.070
1500	9.137	60.890	53.975	10.372	10.154	20.344	-2.964
1600	9.175	61.481	54.426	11.288	10.183	21.022	-2.871
1700	9.211	62.039	54.858	12.207	10.212	21.697	-2.789
1800	9.245	62.566	55.272	13.130	10.237	22.372	-2.716
1900	9.277	63.067	55.669	14.056	10.262	23.046	-2.651
2000	9.308	63.543	56.050	14.985	10.282	23.719	-2.592

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.267 + 0.610\times10^{-3}T - 0.916\times10^{5}T^{-2}$
$H°-H°_{298} = 8.267\times10^{-3}T + 0.305\times10^{-6}T^{2} + 0.916\times10^{2}T^{-1} - 2.799$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = 30.761 + 3.993\times10^{-3}T - 9.972\times10^{-6}T^{2} + 99.850T^{-1}$
$\Delta Gf° = 30.761 - 3.993\times10^{-3}T\ln T + 9.972\times10^{-6}T^{2} + 49.925T^{-1} + 5.115\times10^{-3}T$
336.35-1043.7 K: $\Delta Hf° = 30.764 - 1.806\times10^{-3}T - 0.021\times10^{-6}T^{2} + 188.450T^{-1}$
$\Delta Gf° = 30.764 + 1.806\times10^{-3}T\ln T + 0.021\times10^{-6}T^{2} + 94.225T^{-1} - 25.678\times10^{-3}T$
1043.7-2000 K: $\Delta Hf° = 9.161 + 0.532\times10^{-3}T - 0.027\times10^{-6}T^{2} + 325.450T^{-1}$
$\Delta Gf° = 9.161 - 0.532\times10^{-3}T\ln T + 0.027\times10^{-6}T^{2} + 162.725T^{-1} + 11.201\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data are from JANAF (127).

KHF_2(c,l)
Potassium Hydrogen Fluoride
[Formation: $K(c,l) + 0.5H_2(g) + F_2(g) = KHF_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.390	24.920	24.920	0	-221.720	-205.446	150.594
300	18.429	25.034	24.921	.034	-221.719	-205.345	149.592
336.35	19.155	27.183	25.051	.717	-221.708	-203.362	132.137
336.35	19.155	27.183	25.051	.717	-222.266	-203.362	132.137
400	20.425	30.615	25.667	1.979	-222.204	-199.788	109.158
469.8	21.725	34.002	26.659	3.450	-222.056	-195.888	91.126
469.8	24.466	39.707	26.659	6.130	-219.376	-195.888	91.126
500	24.466	41.231	27.493	6.869	-219.211	-194.383	84.964
511.9	24.466	41.806	27.819	7.160	-219.146	-193.793	82.737
511.9	22.000	44.893	27.819	8.740	-217.566	-193.793	82.737
550	22.000	46.472	29.057	9.578	-217.454	-192.028	76.304

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
469.8 K, α - β transition point of KHF_2; ΔH° = 2.680 kcal/mol.
511.9 K, melting point of KHF_2; ΔH° = 1.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-469.8 K: $Cp^\circ = 13.841 + 17.302\times10^{-3}T - 0.540\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 13.841\times10^{-3}T + 8.651\times10^{-6}T^2 + 0.540\times10^{2}T^{-1} - 5.077$
469.8-511.9 K: $Cp^\circ = 24.466$
$H^\circ - H^\circ_{298} = 24.466\times10^{-3}T - 5.364$
511.9-550 K: $Cp^\circ = 22.000$
$H^\circ - H^\circ_{298} = 22.000\times10^{-3}T - 2.522$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -221.747 + 1.059\times10^{-3}T - 1.800\times10^{-6}T^2 - 38.250T^{-1}$
$\Delta Gf^\circ = -221.747 - 1.059\times10^{-3}T\ln T + 1.800\times10^{-6}T^2 - 19.125T^{-1} + 60.387\times10^{-3}T$
336.35-469.8 K: $\Delta Hf^\circ = -221.744 - 4.740\times10^{-3}T + 8.152\times10^{-6}T^2 + 50.350T^{-1}$
$\Delta Gf^\circ = -221.744 + 4.740\times10^{-3}T\ln T - 8.152\times10^{-6}T^2 + 25.175T^{-1} + 29.594\times10^{-3}T$
469.8-511.9 K: $\Delta Hf^\circ = -222.031 + 5.885\times10^{-3}T - 0.500\times10^{-6}T^2 - 3.650T^{-1}$
$\Delta Gf^\circ = -222.031 - 5.885\times10^{-3}T\ln T + 0.500\times10^{-6}T^2 - 1.825T^{-1} + 91.632\times10^{-3}T$
511.9-550 K: $\Delta Hf^\circ = -219.189 + 3.419\times10^{-3}T - 0.500\times10^{-6}T^2 - 3.650T^{-1}$
$\Delta Gf^\circ = -219.189 - 3.419\times10^{-3}T\ln T + 0.500\times10^{-6}T^2 - 1.825T^{-1} + 70.696\times10^{-3}T$

Sources: Enthalpy of formation from Wagman (516). Transition and fusion data from Davis (110). All other data based on Westrum (530).

$KMg_3AlSi_3O_{10}F_2$(c,l)
Fluorphlogopite Mica

[Formation: K(c,l,g) + 3Mg(c,l,g) + Al(c,l) + 3Si(c,l) + $5O_2$(g) + F_2(g) = $KMg_3AlSi_3O_{10}F_2$(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	81.840	75.900	75.900	0	-1522.000	-1439.493	1055.163
300	82.160	76.410	75.910	.150	-1522.013	-1438.980	1048.283
336.35	86.595	86.060	76.495	3.217	-1522.176	-1428.910	928.450
336.35	86.595	86.060	76.495	3.217	-1522.734	-1428.910	928.450
400	94.360	101.960	79.310	9.060	-1522.685	-1411.168	771.017
500	100.840	123.770	86.070	18.850	-1522.276	-1383.326	604.644
600	105.160	142.550	93.950	29.160	-1521.662	-1355.579	493.763
700	108.450	159.020	102.106	39.840	-1520.973	-1327.961	414.603
800	111.190	173.690	110.153	50.830	-1520.247	-1300.446	355.261
900	113.620	186.930	117.963	62.070	-1519.533	-1273.000	309.123
922	114.113	189.680	119.642	64.575	-1519.372	-1266.987	300.321
922	114.113	189.680	119.642	64.575	-1525.789	-1266.987	300.321
933.61	114.373	191.110	120.522	65.901	-1525.706	-1263.729	295.824
933.61	114.373	191.110	120.522	65.901	-1528.286	-1263.729	295.824
1000	115.860	199.010	125.460	73.550	-1527.774	-1244.913	272.072
1043.7	116.778	203.985	128.644	78.633	-1527.426	-1232.558	258.093
1043.7	116.778	203.985	128.644	78.633	-1546.464	-1232.558	258.093
1100	117.960	210.160	132.669	85.240	-1545.872	-1215.681	241.530
1200	119.980	220.510	139.560	97.140	-1544.781	-1185.713	215.945
1300	121.930	230.190	146.167	109.230	-1543.621	-1155.806	194.306
1363	123.133	235.983	150.178	116.951	-1542.866	-1137.068	182.320
1363	123.133	235.983	150.178	116.951	-1633.616	-1137.068	182.320
1400	123.840	239.290	152.490	121.520	-1632.730	-1123.603	175.400
1500	125.720	247.900	158.567	134.000	-1630.239	-1087.363	158.427
1600	127.570	256.070	164.408	146.660	-1627.622	-1051.260	143.594
1670	128.850	261.560	168.367	155.640	-1625.696	-1026.020	134.272
1670	160.500	305.760	168.367	229.440	-1551.896	-1026.020	134.272
1687	160.500	307.378	169.759	232.163	-1550.891	-1020.675	132.226
1687	160.500	307.378	169.759	232.163	-1587.137	-1020.675	132.226
1700	160.500	308.610	170.816	234.250	-1586.338	-1016.301	130.653
1800	160.500	317.790	178.734	250.300	-1580.216	-982.943	119.344

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.
1670 K, melting point of $KMg_3AlSi_3O_{10}F_2$; ΔH° = 73.800 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1670 K: $Cp^\circ = 100.591 + 17.376\times10^{-3}T - 21.098\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 100.591\times10^{-3}T + 8.688\times10^{-6}T^2 + 21.098\times10^{2}T^{-1} - 37.840$
1670-1800 K: $Cp^\circ = 160.500$
$H^\circ - H^\circ_{298} = 160.500\times10^{-3}T - 38.595$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -1531.366 + 17.829\times10^{-3}T - 11.013\times10^{-6}T^2 + 1499.500T^{-1}$
$\Delta Gf^\circ = -1531.366 - 17.829\times10^{-3}T\ln T + 11.013\times10^{-6}T^2 + 749.750T^{-1} + 398.009\times10^{-3}T$
336.35-922 K: $\Delta Hf^\circ = -1531.363 + 12.030\times10^{-3}T - 1.061\times10^{-6}T^2 + 1588.100T^{-1}$
$\Delta Gf^\circ = -1531.363 - 12.030\times10^{-3}T\ln T + 1.061\times10^{-6}T^2 + 794.050T^{-1} + 367.216\times10^{-3}T$
922-933.61 K: $\Delta Hf^\circ = -1535.334 + 9.432\times10^{-3}T - 0.119\times10^{-6}T^2 + 803.000T^{-1}$
$\Delta Gf^\circ = -1535.334 - 9.432\times10^{-3}T\ln T + 0.119\times10^{-6}T^2 + 401.500T^{-1} + 355.118\times10^{-3}T$
933.61-1043.7 K: $\Delta Hf^\circ = -1536.601 + 6.434\times10^{-3}T + 1.608\times10^{-6}T^2 + 785.600T^{-1}$
$\Delta Gf^\circ = -1536.601 - 6.434\times10^{-3}T\ln T - 1.608\times10^{-6}T^2 + 392.800T^{-1} + 337.595\times10^{-3}T$
1043.7-1363 K: $\Delta Hf^\circ = -1558.204 + 8.772\times10^{-3}T + 1.602\times10^{-6}T^2 + 922.600T^{-1}$
$\Delta Gf^\circ = -1558.204 - 8.772\times10^{-3}T\ln T - 1.602\times10^{-6}T^2 + 461.300T^{-1} + 374.474\times10^{-3}T$
1363-1670 K: $\Delta Hf^\circ = -1659.777 + 11.895\times10^{-3}T + 4.824\times10^{-6}T^2 + 1713.400T^{-1}$
$\Delta Gf^\circ = -1659.777 - 11.895\times10^{-3}T\ln T - 4.824\times10^{-6}T^2 + 856.700T^{-1} + 475.715\times10^{-3}T$
1670-1687 K: $\Delta Hf^\circ = -1660.532 + 71.804\times10^{-3}T - 3.864\times10^{-6}T^2 - 396.400T^{-1}$
$\Delta Gf^\circ = -1660.532 - 71.804\times10^{-3}T\ln T + 3.864\times10^{-6}T^2 - 198.200T^{-1} + 906.595\times10^{-3}T$
1687-1800 K: $\Delta Hf^\circ = -1697.819 + 70.541\times10^{-3}T - 2.811\times10^{-6}T^2 - 100.900T^{-1}$
$\Delta Gf^\circ = -1697.819 - 70.541\times10^{-3}T\ln T + 2.811\times10^{-6}T^2 - 50.450T^{-1} + 921.038\times10^{-3}T$

Source: Data based on Kelley (244).

$KMnO_4(c)$
Potassium Permanganate
[Formation: $K(c,l) + Mn(c) + 2O_2(g) = KMnO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.466	41.000	41.000	0	-200.100	-176.213	129.166
300	28.537	41.177	41.000	.053	-200.098	-176.064	128.261
336.35	29.788	44.510	41.203	1.112	-200.054	-173.155	112.509
336.35	29.788	44.510	41.203	1.112	-200.612	-173.155	112.509
350	30.258	45.704	41.355	1.522	-200.588	-172.043	107.427
400	31.955	49.855	42.160	3.078	-200.459	-167.972	91.775
450	33.676	53.720	43.236	4.718	-200.261	-163.922	79.610
500	35.397	57.355	44.465	6.445	-199.995	-159.896	69.890

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp° = 15.596 + 39.240\times10^{-3}T + 1.040\times10^{5}T^{-2}$

$H°- H°_{298} = 15.596\times10^{-3}T + 19.620\times10^{-6}T^{2} - 1.040\times10^{2}T^{-1} - 6.045$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -198.290 - 5.548\times10^{-3}T + 6.839\times10^{-6}T^{2} - 227.800T^{-1}$

$\Delta Gf° = -198.290 + 5.548\times10^{-3}T\ln T - 6.839\times10^{-6}T^{2} - 113.900T^{-1} + 45.756\times10^{-3}T$

336.35-500 K: $\Delta Hf° = -198.287 - 11.347\times10^{-3}T + 16.791\times10^{-6}T^{2} - 139.200T^{-1}$

$\Delta Gf° = -198.287 + 11.347\times10^{-3}T\ln T - 16.791\times10^{-6}T^{2} - 69.600T^{-1} + 14.962\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (516). All other data from Peters (397).

KNO_2(c,l)
Potassium Nitrite
[Formation: $K(c,l,g) + 0.5N_2(g) + O_2(g) = KNO_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	25.670	36.353	36.353	0	-87.450	-72.246	52.957
300	25.880	36.512	36.353	.048	-87.435	-72.151	52.561
314.7	30.880	37.845	36.390	.458	-87.285	-71.405	49.588
314.7	20.790	38.414	36.390	.637	-87.106	-71.405	49.588
336.35	20.876	39.800	36.565	1.088	-87.049	-70.327	45.696
336.35	20.876	39.800	36.565	1.088	-87.607	-70.327	45.696
400	21.130	43.440	37.377	2.425	-87.430	-67.074	36.647
500	21.530	48.198	39.082	4.558	-87.122	-62.019	27.108
600	21.930	52.159	40.941	6.731	-86.787	-57.030	20.773
700	22.330	55.569	42.792	8.944	-86.431	-52.097	16.265
711	22.370	55.920	42.995	9.190	-86.391	-51.560	15.848
711	24.380	61.532	42.995	13.180	-82.401	-51.560	15.848
800	24.380	64.407	45.219	15.350	-81.907	-47.730	13.039
900	24.380	67.278	47.514	17.788	-81.374	-43.489	10.560
1000	24.380	69.847	49.621	20.226	-80.872	-39.308	8.591
1043.7	24.380	70.890	50.490	21.291	-80.662	-37.495	7.851
1043.7	24.380	70.890	50.490	21.291	-99.700	-37.495	7.851
1100	24.380	72.170	51.566	22.664	-99.304	-34.149	6.785
1200	24.380	74.292	53.374	25.102	-98.611	-28.257	5.146
1300	24.380	76.243	55.058	27.540	-97.930	-22.421	3.769
1400	24.380	78.049	56.636	29.978	-97.264	-16.636	2.597
1500	24.380	79.731	58.120	32.416	-96.607	-10.900	1.588

Phase changes: 314.7 K, α - β transition point of KNO_2; ΔH° = 0.179 kcal/mol.
336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
711 K, melting point of KNO_2; ΔH° = 3.990 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-314.7 K: $Cp° = -46.524 + 242.140\times10^{-3}T$
$H°-H°_{298} = -46.524\times10^{-3}T + 121.070\times10^{-6}T^2 + 3.109$
314.7-711 K: $Cp° = 19.530 + 4.000\times10^{-3}T$
$H°-H°_{298} = 19.530\times10^{-3}T + 2.000\times10^{-6}T^2 - 5.707$
711-1500 K: $Cp° = 24.380$
$H°-H°_{298} = 24.380\times10^{-3}T - 4.154$

Formation equations (kcal/mol):

298.15-314.7 K: $\Delta Hf° = -79.798 - 58.059\times10^{-3}T + 110.204\times10^{-6}T^2 - 41.250T^{-1}$
$\Delta Gf° = -79.798 + 58.059\times10^{-3}T\ln T - 110.204\times10^{-6}T^2 - 20.625T^{-1} - 272.375\times10^{-3}T$
314.7-336.35 K: $\Delta Hf° = -88.614 + 7.995\times10^{-3}T - 8.865\times10^{-6}T^2 - 41.250T^{-1}$
$\Delta Gf° = -88.614 - 7.995\times10^{-3}T\ln T + 8.865\times10^{-6}T^2 - 20.625T^{-1} + 98.085\times10^{-3}T$
336.35-711 K: $\Delta Hf° = -88.611 + 2.197\times10^{-3}T + 1.087\times10^{-6}T^2 + 47.350T^{-1}$
$\Delta Gf° = -88.611 - 2.197\times10^{-3}T\ln T - 1.087\times10^{-6}T^2 + 23.675T^{-1} + 67.291\times10^{-3}T$
711-1043.7 K: $\Delta Hf° = -87.058 + 7.046\times10^{-3}T - 0.914\times10^{-6}T^2 + 47.350T^{-1}$
$\Delta Gf° = -87.058 - 7.046\times10^{-3}T\ln T + 0.914\times10^{-6}T^2 + 23.675T^{-1} + 95.534\times10^{-3}T$
1043.7-1500 K: $\Delta Hf° = -108.661 + 9.384\times10^{-3}T - 0.919\times10^{-6}T^2 + 184.350T^{-1}$
$\Delta Gf° = -108.661 - 9.384\times10^{-3}T\ln T + 0.919\times10^{-6}T^2 + 92.175T^{-1} + 132.414\times10^{-3}T$

Source: Data from Gurvich (193).

$KNO_3(c,l)$
Potassium Nitrate
[Formation: $K(c,l) + 0.5N_2(g) + 1.5O_2(g) = KNO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	22.802	31.800	31.800	0	-118.220	-94.353	69.162
300	22.868	31.941	31.801	.042	-118.217	-94.205	68.627
336.35	24.206	34.633	31.964	.898	-118.144	-91.300	59.323
336.35	24.206	34.633	31.964	.898	-118.702	-91.300	59.323
400	26.550	39.015	32.740	2.510	-118.477	-86.132	47.060
406	26.787	39.412	32.836	2.670	-118.447	-85.647	46.103
406	30.201	42.614	32.836	3.970	-117.147	-85.647	46.103
500	30.282	48.818	35.276	6.771	-116.407	-78.433	34.283
600	33.734	54.602	38.020	9.949	-115.444	-70.923	25.833
610	34.036	55.162	38.297	10.288	-115.328	-70.182	25.144
610	33.624	59.097	38.297	12.688	-112.928	-70.182	25.144
700	33.450	63.713	41.276	15.706	-111.933	-63.946	19.965
800	33.256	68.166	44.364	19.042	-110.878	-57.164	15.616

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
406 K, α - β transition point of KNO_3; ΔH° = 1.300 kcal/mol.
610 K, melting point of KNO_3; ΔH° = 2.400 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-406 K: $Cp° = 9.514 + 41.198x10^{-3}T + 0.893x10^{5}T^{-2}$
$H°-H°_{298} = 9.514x10^{-3}T + 20.599x10^{-6}T^{2} - 0.893x10^{2}T^{-1} - 4.368$
406-610 K: $Cp° = -24.966 + 80.828x10^{-3}T + 36.843x10^{5}T^{-2}$
$H°-H°_{298} = -24.966x10^{-3}T + 40.414x10^{-6}T^{2} - 36.843x10^{2}T^{-1} + 16.519$
610-800 K: $Cp° = 34.084 - 1.214x10^{-3}T + 1.044x10^{5}T^{-2}$
$H°-H°_{298} = 34.084x10^{-3}T - 0.607x10^{-6}T^{2} - 1.044x10^{2}T^{-1} - 7.706$

Formation equations (kcal/mol):

298.15-336.35 K: $ΔHf° = -116.869 - 5.635x10^{-3}T + 9.482x10^{-6}T^{2} - 153.150T^{-1}$
$ΔGf° = -116.869 + 5.635x10^{-3}TlnT - 9.482x10^{-6}T^{2} - 76.575T^{-1} + 47.098x10^{-3}T$
336.35-406 K: $ΔHf° = -116.866 - 11.434x10^{-3}T + 19.434x10^{-6}T^{2} - 64.550T^{-1}$
$ΔGf° = -116.866 + 11.434x10^{-3}TlnT - 19.434x10^{-6}T^{2} - 32.275T^{-1} + 16.305x10^{-3}T$
406-610 K: $ΔHf° = -95.978 - 45.915x10^{-3}T + 39.249x10^{-6}T^{2} - 3659.550T^{-1}$
$ΔGf° = -95.978 + 45.915x10^{-3}TlnT - 39.249x10^{-6}T^{2} - 1829.775T^{-1} - 223.291x10^{-3}T$
610-800 K: $ΔHf° = -120.204 + 13.135x10^{-3}T - 1.772x10^{-6}T^{2} - 79.650T^{-1}$
$ΔGf° = -120.204 - 13.135x10^{-3}TlnT + 1.772x10^{-6}T^{2} - 39.825T^{-1} + 165.304x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Southard (471). High-temperature data based on Carling (69), Ichikawa (212), and Schmidt (448).

KOH(c,l)
Potassium Hydroxide
[Formation: $K(c,l,g) + 0.5O_2(g) + 0.5H_2(g) = KOH(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	15.510	18.850	18.850	0	-101.521	-90.575	66.392
300	15.527	18.946	18.850	.029	-101.518	-90.507	65.933
336.35	16.025	20.750	18.959	.602	-101.469	-89.176	57.943
336.35	16.025	20.750	18.959	.602	-102.027	-89.176	57.943
400	16.898	23.581	19.473	1.643	-101.920	-86.752	47.399
500	19.009	27.566	20.700	3.433	-101.588	-82.994	36.276
522.15	19.568	28.402	21.010	3.860	-101.483	-82.173	34.394
522.15	16.946	31.227	21.010	5.335	-100.008	-82.173	34.394
600	20.771	33.841	22.503	6.803	-99.672	-79.533	28.970
683.15	24.856	36.797	24.062	8.700	-98.985	-76.785	24.564
683.15	20.400	39.468	24.062	10.525	-97.160	-76.785	24.564
700	20.400	39.965	24.438	10.869	-97.062	-76.283	23.816
800	20.400	42.689	26.553	12.909	-96.486	-73.355	20.039
900	20.400	45.092	28.482	14.949	-95.920	-70.497	17.119
1000	20.400	47.241	30.252	16.989	-95.374	-67.703	14.796
1043.7	20.400	48.114	30.982	17.880	-95.142	-66.497	13.924
1043.7	20.400	48.114	30.982	17.880	-114.180	-66.497	13.924
1100	20.400	49.185	31.886	19.029	-113.753	-63.936	12.703
1200	20.400	50.960	33.403	21.069	-113.002	-59.439	10.825
1300	20.400	52.593	34.817	23.109	-112.259	-55.006	9.247

Phase changes:
336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
522.15 K, α - β transition point of KOH; ΔH° = 1.475 kcal/mol.
683.15 K, melting point of KOH; ΔH° = 1.825 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-522.15 K: $Cp° = 5.119 + 25.760\times10^{-3}T + 2.410\times10^{5}T^{-2}$
$H°-H°_{298} = 5.119\times10^{-3}T + 12.880\times10^{-6}T^{2} - 2.410\times10^{2}T^{-1} - 1.863$
522.15-683.15 K: $Cp° = -8.707 + 49.130\times10^{-3}T$
$H°-H°_{298} = -8.707\times10^{-3}T + 24.565\times10^{-6}T^{2} + 3.184$
683.15-1300 K: $Cp° = 20.400$
$H°-H°_{298} = 20.400\times10^{-3}T - 3.411$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -100.048 - 2.770\times10^{-3}T + 2.351\times10^{-6}T^{2} - 255.350T^{-1}$
$\Delta Gf° = -100.048 + 2.770\times10^{-3}T\ln T - 2.351\times10^{-6}T^{2} - 127.675T^{-1} + 18.126\times10^{-3}T$
336.35-522.15 K: $\Delta Hf° = -100.044 - 8.569\times10^{-3}T + 12.303\times10^{-6}T^{2} - 166.750T^{-1}$
$\Delta Gf° = -100.044 + 8.569\times10^{-3}T\ln T - 12.303\times10^{-6}T^{2} - 83.375T^{-1} - 12.667\times10^{-3}T$
522.15-683.15 K: $\Delta Hf° = -94.998 - 22.395\times10^{-3}T + 23.988\times10^{-6}T^{2} + 74.250T^{-1}$
$\Delta Gf° = -94.998 + 22.395\times10^{-3}T\ln T - 23.988\times10^{-6}T^{2} + 37.125T^{-1} - 103.196\times10^{-3}T$
683.15-1043.7 K: $\Delta Hf° = -101.593 + 6.712\times10^{-3}T - 0.577\times10^{-6}T^{2} + 74.250T^{-1}$
$\Delta Gf° = -101.593 - 6.712\times10^{-3}T\ln T + 0.577\times10^{-6}T^{2} + 37.125T^{-1} + 79.650\times10^{-3}T$
1043.7-1300 K: $\Delta Hf° = -123.196 + 9.050\times10^{-3}T - 0.583\times10^{-6}T^{2} + 211.250T^{-1}$
$\Delta Gf° = -123.196 - 9.050\times10^{-3}T\ln T + 0.583\times10^{-6}T^{2} + 105.625T^{-1} + 116.529\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Stull (478). High-temperature data based on Powers (407) and Ginzburg (173, 174).

KOH(g)
Potassium Hydroxide (ideal gas)
[Formation: K(c,l,g) + 0.5O_2(g) + 0.5H_2(g) = KOH(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	11.599	56.469	56.469	0	-54.500	-54.770	40.147
300	11.613	56.541	56.471	.021	-54.505	-54.772	39.901
336.35	11.803	57.880	56.552	.447	-54.604	-54.799	35.606
336.35	11.803	57.880	56.552	.447	-55.162	-54.799	35.606
400	12.136	59.962	56.932	1.212	-55.330	-54.715	29.894
500	12.407	62.703	57.823	2.440	-55.560	-54.535	23.837
600	12.578	64.981	58.831	3.690	-55.764	-54.309	19.782
700	12.712	66.930	59.851	4.955	-55.955	-54.051	16.875
800	12.835	68.635	60.845	6.232	-56.142	-53.768	14.688
900	12.959	70.154	61.796	7.522	-56.326	-53.459	12.981
1000	13.083	71.526	62.702	8.824	-56.517	-53.131	11.612
1043.7	13.137	72.087	63.083	9.397	-56.604	-52.981	11.094
1043.7	13.137	72.087	63.083	9.397	-75.642	-52.981	11.094
1100	13.207	72.779	63.562	10.139	-75.622	-51.759	10.283
1200	13.327	73.933	64.379	11.465	-75.585	-49.590	9.031
1300	13.442	75.004	65.155	12.804	-75.543	-47.425	7.973
1400	13.551	76.005	65.895	14.154	-75.500	-45.263	7.066
1500	13.652	76.943	66.600	15.514	-75.456	-43.105	6.280
1600	13.746	77.827	67.275	16.884	-75.411	-40.951	5.594
1700	13.832	78.663	67.920	18.263	-75.363	-38.798	4.988
1800	13.911	79.456	68.539	19.650	-75.318	-36.649	4.450
1900	13.983	80.210	69.134	21.045	-75.272	-34.501	3.969
2000	14.048	80.929	69.706	22.446	-75.229	-32.357	3.536

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 12.244 + 0.946\text{x}10^{-3}T - 0.824\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 12.244\text{x}10^{-3}T + 0.473\text{x}10^{-6}T^2 + 0.824\text{x}10^{2}T^{-1} - 3.969$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -55.133 + 4.355\text{x}10^{-3}T - 10.056\text{x}10^{-6}T^2 + 68.050T^{-1}$
$\Delta Gf^\circ = -55.133 - 4.355\text{x}10^{-3}T\ln T + 10.056\text{x}10^{-6}T^2 + 34.025T^{-1} + 22.648\text{x}10^{-3}T$
336.35-1043.7 K: $\Delta Hf^\circ = -55.130 - 1.444\text{x}10^{-3}T - 0.104\text{x}10^{-6}T^2 + 156.650T^{-1}$
$\Delta Gf^\circ = -55.130 + 1.444\text{x}10^{-3}T\ln T + 0.104\text{x}10^{-6}T^2 + 78.325T^{-1} - 8.145\text{x}10^{-3}T$
1043.7-2000 K: $\Delta Hf^\circ = -76.732 + 0.894\text{x}10^{-3}T - 0.110\text{x}10^{-6}T^2 + 293.650T^{-1}$
$\Delta Gf^\circ = -76.732 - 0.894\text{x}10^{-3}T\ln T + 0.110\text{x}10^{-6}T^2 + 146.825T^{-1} + 28.735\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Farber (142). Other data from Chase (81) who estimated some molecular constants.

$(KOH)_2(g)$
Dimeric Potassium Hydroxide (ideal gas)
[Formation: $2K(c,l,g) + O_2(g) + H_2(g) = (KOH)_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.465	78.366	78.366	0	-156.500	-146.733	107.557
300	19.496	78.487	78.367	.036	-156.516	-146.672	106.849
336.35	20.069	80.750	78.505	.755	-156.846	-145.460	94.514
336.35	20.069	80.750	78.505	.755	-157.962	-145.460	94.514
400	21.073	84.315	79.150	2.066	-158.518	-143.044	78.154
500	22.452	89.170	80.682	4.244	-159.256	-139.087	60.794
600	23.578	93.366	82.453	6.548	-159.859	-134.993	49.171
700	24.488	97.072	84.283	8.952	-160.367	-130.809	40.840
800	25.329	100.392	86.092	11.440	-160.807	-126.557	34.573
900	25.879	103.403	87.851	13.997	-161.199	-122.251	29.686
1000	26.435	106.159	89.546	16.613	-161.570	-117.905	25.768
1043.7	26.649	107.294	90.266	17.773	-161.730	-115.992	24.288
1043.7	26.649	107.294	90.266	17.773	-199.806	-115.992	24.288
1100	26.925	108.702	91.174	19.281	-199.741	-111.473	22.147
1200	27.362	111.063	92.733	21.996	-199.604	-103.450	18.841
1300	27.751	113.269	94.229	24.752	-199.442	-95.445	16.045
1400	28.100	115.339	95.664	27.545	-199.263	-87.451	13.651
1500	28.412	117.288	97.041	30.371	-199.068	-79.470	11.579
1600	28.692	119.131	98.365	33.226	-198.863	-71.506	9.767
1700	28.943	120.878	99.638	36.108	-198.644	-63.552	8.170
1800	29.168	122.539	100.865	39.014	-198.421	-55.613	6.752
1900	29.370	124.122	102.048	41.941	-198.192	-47.685	5.485
2000	29.552	125.633	103.190	44.887	-197.962	-39.770	4.346

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.838 + 4.534\times10^{-3}T - 3.311\times10^{5}T^{-2}$
$H° - H°_{298} = 21.838\times10^{-3}T + 2.267\times10^{-6}T^{2} + 3.311\times10^{2}T^{-1} - 7.823$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -157.651 + 6.060\times10^{-3}T - 18.791\times10^{-6}T^{2} + 302.400T^{-1}$
$\Delta Gf° = -157.651 - 6.060\times10^{-3}T\ln T + 18.791\times10^{-6}T^{2} + 151.200T^{-1} + 63.843\times10^{-3}T$
336.35-1043.7 K: $\Delta Hf° = -157.644 - 5.538\times10^{-3}T + 1.113\times10^{-6}T^{2} + 479.600T^{-1}$
$\Delta Gf° = -157.644 + 5.538\times10^{-3}T\ln T - 1.113\times10^{-6}T^{2} + 239.800T^{-1} + 2.257\times10^{-3}T$
1043.7-2000 K: $\Delta Hf° = -200.850 - 0.862\times10^{-3}T + 1.101\times10^{-6}T^{2} + 753.600T^{-1}$
$\Delta Gf° = -200.850 + 0.862\times10^{-3}T\ln T - 1.101\times10^{-6}T^{2} + 376.800T^{-1} + 76.016\times10^{-3}T$

Source: Data from Chase (81) who estimated all except enthalpy of formation at 298 K.

K_2SO_4(c,l)
Potassium Sulfate
[Reaction: $2K(c,l,g) + 0.5S_2(g) + 2O_2(g) = K_2SO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	31.386	41.956	41.956	0	-358.975	-324.920	238.170
300	31.469	42.150	41.957	.058	-358.976	-324.708	236.546
336.35	32.858	45.829	42.180	1.227	-359.004	-320.554	208.284
336.35	32.858	45.829	42.180	1.227	-360.120	-320.554	208.284
400	35.289	51.743	43.238	3.402	-360.079	-313.070	171.051
500	38.416	59.959	45.779	7.090	-359.753	-301.348	131.718
600	41.235	67.205	48.758	11.068	-359.160	-289.718	105.528
700	44.543	73.812	51.872	15.358	-358.289	-278.209	86.860
800	47.710	79.966	55.002	19.971	-357.132	-266.847	72.898
857	49.515	83.312	56.775	22.742	-356.345	-260.441	66.416
857	43.977	85.669	56.775	24.762	-354.325	-260.441	66.416
900	44.810	87.842	58.208	26.671	-353.923	-255.740	62.101
1000	46.750	92.663	61.414	31.249	-352.885	-244.886	53.519
1043.7	47.602	94.681	62.765	33.311	-352.387	-240.175	50.292
1043.7	47.602	94.681	62.765	33.311	-390.463	-240.175	50.292
1100	48.700	97.211	64.465	36.021	-389.513	-232.094	46.112
1200	50.640	101.531	67.374	40.988	-387.686	-217.859	39.677
1300	52.580	105.661	70.162	46.149	-385.684	-203.788	34.259
1342	53.390	107.346	71.299	48.375	-384.791	-197.925	32.232
1342	48.150	113.471	71.299	56.595	-376.571	-197.925	32.232
1400	48.150	115.509	73.090	59.387	-375.626	-190.224	29.695
1500	48.150	118.831	76.030	64.202	-374.008	-177.039	25.794
1600	48.150	121.938	78.802	69.017	-372.408	-163.960	22.396
1700	48.150	124.857	81.426	73.832	-370.820	-150.981	19.410
1800	48.150	127.609	83.916	78.647	-369.251	-138.093	16.767
1900	48.150	130.213	86.286	83.462	-367.698	-125.295	14.412
2000	48.150	132.682	88.544	88.277	-366.161	-112.576	12.302

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
857 K, α - β transition point of K_2SO_4; ΔH° = 2.020 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1342 K, melting point of K_2SO_4; ΔH° = 8.220 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-857 K: $Cp° = 24.304 + 29.390x10^{-3}T - 1.494x10^{5}T^{-2}$
$H°-H°_{298} = 24.304x10^{-3}T + 14.695x10^{-6}T^{2} + 1.494x10^{2}T^{-1} - 9.054$
857-1342 K: $Cp° = 27.143 + 19.546x10^{-3}T + 0.612x10^{5}T^{-2}$
$H°-H°_{298} = 27.143x10^{-3}T + 9.773x10^{-6}T^{2} - 0.612x10^{2}T^{-1} - 5.606$
1342-2000 K: $Cp° = 48.150$
$H°-H°_{298} = 48.150x10^{-3}T - 8.022$

Reaction equations (kcal/mol):

298.15-336.35 K: $ΔHr° = -359.539 + 3.580x10^{-3}T - 6.607x10^{-6}T^{2} + 24.850T^{-1}$
$ΔGr° = -359.539 - 3.580x10^{-3}TlnT + 6.607x10^{-6}T^{2} + 12.425T-1 + 134.402x10^{-3}T$
336.35-857 K: $ΔHr° = -359.532 - 8.018x10^{-3}T + 13.297x10^{-6}T^{2} + 202.050T^{-1}$
$ΔGr° = -359.532 + 8.018x10^{-3}TlnT - 13.297x10^{-6}T^{2} + 101.025T^{-1} + 72.815x10^{-3}T$
857-1043.7 K: $ΔHr° = -356.084 - 5.179x10^{-3}T + 8.375x10^{-6}T^{2} - 8.550T^{-1}$
$ΔGr° = -356.084 + 5.179x10^{-3}TlnT - 8.375x10^{-6}T^{2} - 4.275T^{-1} + 83.891x10^{-3}T$
1043.7-1342 K: $ΔHr° = -399.290 - 0.503x10^{-3}T + 8.363x10^{-6}T^{2} + 265.450T^{-1}$
$ΔGr° = -399.290 + 0.503x10^{-3}TlnT - 8.363x10^{-6}T^{2} + 132.725T^{-1} + 157.650x10^{-3}T$
1342-2000 K: $ΔHr° = -401.706 + 20.505x10^{-3}T - 1.410x10^{-6}T^{2} + 326.650T^{-1}$
$ΔGr° = -401.706 - 20.505x10^{-3}TlnT + 1.410x10^{-6}T^{2} + 163.325T^{-1} + 297.608x10^{-3}T$

Source: Data from Chase (80).

$K_2SO_4(g)$
Potassium Sulfate (ideal gas)
[Reaction: $2K(c,l,g) + 0.5S_2(g) + 2O_2(g) = K_2SO_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	25.987	87.486	87.486	0	-276.855	-256.375	187.925
300	26.057	87.647	87.487	.048	-276.866	-256.247	186.673
336.35	27.214	90.693	87.672	1.016	-277.095	-253.736	164.867
336.35	27.214	90.693	87.672	1.016	-278.211	-253.736	164.867
400	29.240	95.607	88.552	2.822	-278.539	-249.075	136.087
500	31.442	102.383	90.657	5.863	-278.859	-241.667	105.631
600	32.960	108.259	93.112	9.088	-279.021	-234.211	85.310
700	34.021	113.424	95.653	12.440	-279.087	-226.736	70.789
800	34.781	118.019	98.166	15.882	-279.100	-219.258	59.898
900	35.339	122.149	100.605	19.390	-279.085	-211.777	51.426
1000	35.758	125.896	102.950	22.946	-279.068	-204.301	44.649
1043.7	35.898	127.428	103.943	24.512	-279.066	-201.033	42.096
1043.7	35.898	127.428	103.943	24.512	-317.142	-201.033	42.096
1100	36.079	129.319	105.194	26.538	-316.876	-194.776	38.698
1200	36.330	132.470	107.338	30.159	-316.396	-183.695	33.455
1300	36.530	135.386	109.384	33.803	-315.910	-172.657	29.026
1400	36.691	138.099	111.339	37.464	-315.430	-161.653	25.235
1500	36.823	140.635	113.208	41.140	-314.949	-150.687	21.955
1600	36.932	143.015	114.997	44.828	-314.477	-139.752	19.089
1700	37.023	145.257	116.712	48.526	-314.007	-128.847	16.564
1800	37.100	147.376	118.358	52.232	-313.547	-117.968	14.323
1900	37.165	149.383	119.938	55.945	-313.095	-107.115	12.321
2000	37.222	151.291	121.459	59.665	-312.654	-96.285	10.521

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:
$Cp° = 33.687 + 2.326\times10^{-3}T - 7.461\times10^{5}T^{-2}$
$H°- H^\circ_{298} = 33.687\times10^{-3}T + 1.163\times10^{-6}T^{2} + 7.461\times10^{2}T^{-1} - 12.650$

Reaction equations (kcal/mol):

298.15-336.35 K:
$\Delta Hr° = -281.015 + 12.963\times10^{-3}T - 20.139\times10^{-6}T^{2} + 621.550T^{-1}$
$\Delta Gr° = -281.015 - 12.963\times10^{-3}T\ln T + 20.139\times10^{-6}T^{2} + 310.775T^{-1} + 147.002\times10^{-3}T$

336.35-1043.7 K:
$\Delta Hr° = -281.008 + 1.365\times10^{-3}T - 0.235\times10^{-6}T^{2} + 798.750T^{-1}$
$\Delta Gr° = -281.008 - 1.365\times10^{-3}T\ln T + 0.235\times10^{-6}T^{2} + 399.375T^{-1} + 85.416\times10^{-3}T$

1043.7-2000 K:
$\Delta Hr° = -324.214 + 6.041\times10^{-3}T - 0.247\times10^{-6}T^{2} + 1072.750T^{-1}$
$\Delta Gr° = -324.214 - 6.041\times10^{-3}T\ln T + 0.247\times10^{-6}T^{2} + 536.375T^{-1} + 159.175\times10^{-3}T$

Source: Data from Chase (80).

$K_2SiO_3(c)$
Potassium Silicate
[Formation: $2K(c,l,g) + Si(c) + 1.5O_2(g) = K_2SiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	28.100	34.930	34.930	0	-370.000	-347.939	255.043
300	28.170	35.104	34.931	.052	-370.003	-347.802	253.370
336.35	29.188	38.384	35.130	1.094	-370.064	-345.109	224.238
336.35	29.188	38.384	35.130	1.094	-371.180	-345.109	224.238
400	30.970	43.620	36.070	3.020	-371.234	-340.171	185.858
500	32.900	50.750	38.314	6.218	-371.165	-332.409	145.294
600	34.480	56.890	40.908	9.589	-370.951	-324.675	118.261
700	35.890	62.320	43.591	13.110	-370.620	-316.991	98.968
800	37.220	67.200	46.244	16.765	-370.191	-309.360	84.512
900	38.500	71.650	48.817	20.550	-369.671	-301.779	73.281
1000	39.750	75.780	51.315	24.465	-369.066	-294.267	64.311
1043.7	40.283	77.492	52.375	26.214	-368.780	-291.003	60.935
1043.7	40.283	77.492	52.375	26.214	-406.856	-291.003	60.935
1100	40.970	79.620	53.711	28.500	-406.201	-284.773	56.578
1200	42.180	83.240	56.028	32.655	-404.956	-273.793	49.864
1249	42.770	84.940	57.126	34.740	-404.303	-268.447	46.972

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1249 K, melting point of K_2SiO_3. On cooling, liquid solidifies to a mixture of crystalline and vitreous forms.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1249 K:
$$Cp° = 28.418 + 11.666\times10^{-3}T - 3.383\times10^{5}T^{-2}$$
$$H°-H°_{298} = 28.418\times10^{-3}T + 5.833\times10^{-6}T^{2} + 3.383\times10^{2}T^{-1} - 10.126$$

Formation equations (kcal/mol):

298.15-336.35 K:
$$\Delta Hf° = -372.130 + 9.802\times10^{-3}T - 15.408\times10^{-6}T^{2} + 172.000T^{-1}$$
$$\Delta Gf° = -372.130 - 9.802\times10^{-3}T\ln T + 15.408\times10^{-6}T^{2} + 86.000T^{-1} + 131.421\times10^{-3}T$$

336.35-1043.7 K:
$$\Delta Hf° = -372.123 - 1.796\times10^{-3}T + 4.496\times10^{-6}T^{2} + 349.200T^{-1}$$
$$\Delta Gf° = -372.123 + 1.796\times10^{-3}T\ln T - 4.496\times10^{-6}T^{2} + 174.600T^{-1} + 69.834\times10^{-3}T$$

1043.7-1249 K:
$$\Delta Hf° = -415.329 + 2.880\times10^{-3}T + 4.484\times10^{-6}T^{2} + 623.200T^{-1}$$
$$\Delta Gf° = -415.329 - 2.880\times10^{-3}T\ln T - 4.484\times10^{-6}T^{2} + 311.600T^{-1} + 143.593\times10^{-3}T$$

Source: Data from Beyer (42).

$K_2Si_2O_5(c,l)$
Potassium Disilicate
[Formation: $2K(c,l,g) + 2Si(c) + 2.5O_2(g) = K_2Si_2O_5(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$C_p°$	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	38.407	45.550	45.550	0	-599.400	-564.553	413.823
300	38.522	45.788	45.551	.071	-599.406	-564.337	411.114
336.35	40.441	50.303	45.826	1.506	-599.508	-560.082	363.919
336.35	40.441	50.303	45.826	1.506	-600.624	-560.082	363.919
400	43.800	57.700	47.143	4.223	-600.671	-552.411	301.819
500	46.670	67.800	50.286	8.757	-600.542	-540.351	236.184
510	46.900	68.730	50.642	9.225	-600.519	-539.149	231.038
510	47.920	69.300	50.642	9.515	-600.229	-539.149	231.038
600	50.130	77.260	54.043	13.930	-599.853	-528.397	192.466
700	52.470	85.170	57.941	19.060	-599.282	-516.536	161.268
800	54.760	92.320	61.795	24.420	-598.551	-504.760	137.892
867	56.270	96.790	64.334	28.140	-597.972	-496.932	125.263
867	54.510	97.230	64.334	28.520	-597.592	-496.932	125.263
900	54.540	99.260	65.571	30.320	-597.350	-493.099	119.739
1000	54.650	105.000	69.220	35.780	-596.655	-481.526	105.236
1043.7	54.694	107.338	70.767	38.169	-596.372	-476.499	99.777
1043.7	54.694	107.338	70.767	38.169	-634.448	-476.499	99.777
1100	54.750	110.200	72.700	41.250	-633.831	-467.996	92.981
1200	54.860	115.000	76.058	46.730	-632.753	-453.005	82.502
1300	54.960	119.400	79.231	52.220	-631.695	-438.077	73.647
1318	54.980	120.100	79.734	53.210	-631.506	-435.331	72.185
1318	65.800	126.500	79.734	61.630	-623.086	-435.331	72.185
1400	65.800	130.500	82.621	67.030	-621.353	-423.736	66.147
1500	65.800	135.000	85.927	73.610	-619.268	-409.657	59.686
1600	65.800	139.300	89.181	80.190	-617.212	-395.840	54.069

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
510 K, α - β transition point of $K_2Si_2O_5$; ΔH° = 0.290 kcal/mol.
867 K, β - γ transition point of $K_2Si_2O_5$; ΔH° = 0.380 kcal/mol.
1043.7 K, boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1318 K, melting point of $K_2Si_2O_5$; ΔH° = 8.420 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-510 K: $C_p° = 45.855 + 8.744\times10^{-3}T - 8.883\times10^{5}T^{-2}$
$H°- H°_{298} = 45.855\times10^{-3}T + 4.372\times10^{-6}T^2 + 8.883\times10^{2}T^{-1} - 17.040$
510-867 K: $C_p° = 38.042 + 21.410\times10^{-3}T - 2.711\times10^{5}T^{-2}$
$H°- H°_{298} = 38.042\times10^{-3}T + 10.705\times10^{-6}T^2 + 2.711\times10^{2}T^{-1} - 13.202$
867-1318 K: $C_p° = 53.591 + 1.056\times10^{-3}T$
$H°- H°_{298} = 53.591\times10^{-3}T + 0.528\times10^{-6}T^2 - 18.340$
1318-1600 K: $C_p° = 65.800$
$H°- H°_{298} = 65.800\times10^{-3}T - 25.094$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -604.037 + 14.330\times10^{-3}T - 17.724\times10^{-6}T^2 + 578.300T^{-1}$
$\Delta Gf° = -604.037 - 14.330\times10^{-3}T\ln T + 17.724\times10^{-6}T^2 + 289.150T^{-1} + 205.537\times10^{-3}T$
336.35-510 K: $\Delta Hf° = -604.030 + 2.732\times10^{-3}T + 2.181\times10^{-6}T^2 + 755.500T^{-1}$
$\Delta Gf° = -604.030 - 2.732\times10^{-3}T\ln T - 2.181\times10^{-6}T^2 + 377.750T^{-1} + 143.951\times10^{-3}T$
510-867 K: $\Delta Hf° = -600.193 - 5.081\times10^{-3}T + 8.514\times10^{-6}T^2 + 138.300T^{-1}$
$\Delta Gf° = -600.193 + 5.081\times10^{-3}T\ln T - 8.514\times10^{-6}T^2 + 69.150T^{-1} + 92.133\times10^{-3}T$
867-1043.7 K: $\Delta Hf° = -605.331 + 10.468\times10^{-3}T - 1.664\times10^{-6}T^2 - 132.800T^{-1}$
$\Delta Gf° = -605.331 - 10.458\times10^{-3}T\ln T + 1.664\times10^{-6}T^2 - 66.400T^{-1} + 194.606\times10^{-3}T$
1043.7-1318 K: $\Delta Hf° = -648.537 + 15.144\times10^{-3}T - 1.676\times10^{-6}T^2 + 141.200T^{-1}$
$\Delta Gf° = -648.537 - 15.144\times10^{-3}T\ln T + 1.676\times10^{-6}T^2 + 70.600T^{-1} + 268.365\times10^{-3}T$
1318-1600 K: $\Delta Hf° = -655.291 + 27.353\times10^{-3}T - 2.204\times10^{-6}T^2 + 141.200T^{-1}$
$\Delta Gf° = -655.291 - 27.353\times10^{-3}T\ln T + 2.204\times10^{-6}T^2 + 70.600T^{-1} + 360.502\times10^{-3}T$

Source: Data from Beyer (42).

$K_2Si_2O_5$(vitreous)
Potassium Disilicate
[Formation: $2K(c,l) + 2Si(c) + 2.5O_2(g) = K_2Si_2O_5(vit)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	38.400	48.950	48.950	0	-594.900	-561.067	411.268
300	38.550	49.190	48.957	.070	-594.906	-560.858	408.580
336.35	40.611	53.717	49.231	1.509	-595.006	-556.727	361.740
336.35	40.611	53.717	49.231	1.509	-596.122	-556.727	361.740
400	44.220	61.140	50.540	4.240	-596.154	-549.270	300.103
500	47.620	71.400	53.720	8.840	-595.959	-537.568	234.968
600	50.130	80.310	57.418	13.735	-595.548	-525.922	191.565
700	52.220	88.200	61.264	18.855	-594.987	-514.362	160.589
800	54.080	95.290	65.077	24.170	-594.301	-502.886	137.380
900	55.820	101.770	68.809	29.665	-593.505	-491.513	119.354

Phase change: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp° = 43.807 + 14.536\times10^{-3}T - 8.649\times10^{5}T^{-2}$
$H°-H°_{298} = 43.807\times10^{-3}T + 7.268\times10^{-6}T^{2} + 8.649\times10^{2}T^{-1} - 16.608$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -599.105 + 12.282\times10^{-3}T - 14.828\times10^{-6}T^{2} + 554.900T^{-1}$
$\Delta Gf° = -599.105 - 12.282\times10^{-3}T\ln T + 14.828\times10^{-6}T^{2} + 277.450T^{-1} + 190.016\times10^{-3}T$
336.35-900 K: $\Delta Hf° = -599.099 + 0.684\times10^{-3}T + 5.077\times10^{-6}T^{2} + 732.100T^{-1}$
$\Delta Gf° = -599.099 - 0.684\times10^{-3}T\ln T - 5.077\times10^{-6}T^{2} + 366.050T^{-1} + 128.429\times10^{-3}T$

Source: Data from Beyer (42).

$LaB_6(c)$
Lanthanum Hexaboride
[Formation: $La(c,l) + 6B(\beta) = LaB_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	23.160	19.870	19.870	0	-95.700	-95.047	69.670
300	23.230	20.010	19.877	.040	-95.702	-95.039	69.235
400	28.830	27.560	20.860	2.680	-95.616	-94.844	51.820
500	31.970	34.360	22.900	5.730	-95.665	-94.635	41.364
550	33.070	37.465	24.085	7.359	-95.760	-94.544	37.568
550	33.070	37.465	24.085	7.359	-95.847	-94.544	37.568
600	34.170	40.390	25.323	9.040	-95.951	-94.421	34.392
700	35.950	45.790	27.861	12.550	-96.227	-94.127	29.387
800	37.530	50.700	30.413	16.230	-96.531	-93.803	25.625
900	39.000	55.200	32.922	20.050	-96.865	-93.445	22.691
1000	40.430	59.390	35.370	24.020	-97.196	-93.046	20.335
1100	41.840	63.310	37.728	28.140	-97.507	-92.645	18.407
1134	42.319	64.591	38.514	29.571	-97.612	-92.495	17.826
1134	42.319	64.591	38.514	29.571	-98.358	-92.495	17.826
1193	43.151	66.757	39.861	32.088	-98.598	-92.176	16.886
1193	43.151	66.757	39.861	32.088	-100.079	-92.176	16.886
1200	43.250	67.010	40.018	32.390	-100.096	-92.128	16.779
1300	44.680	70.530	42.230	36.790	-100.320	-91.441	15.372
1400	46.130	73.890	44.369	41.330	-100.488	-90.744	14.166
1500	47.600	77.120	46.447	46.010	-100.606	-90.016	13.115
1600	49.100	80.240	48.459	50.850	-100.654	-89.374	12.208
1700	50.640	83.260	50.413	55.840	-100.636	-88.668	11.399
1800	52.210	86.200	52.322	60.980	-100.552	-87.898	10.672
1900	53.820	89.070	54.186	66.280	-100.392	-87.187	10.029
2000	55.460	91.870	56.000	71.740	-100.156	-86.576	9.460

*Data extrapolated 298 to 1100 K.

Phase changes: 550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2200 K: $Cp° = 28.316 + 13.224\times10^{-3}T - 8.088\times10^{5}T^{-2}$
$H°-H°_{298} = 28.316\times10^{-3}T + 6.612\times10^{-6}T^{2} + 8.088\times10^{2}T^{-1} - 11.743$

Formation equations (kcal/mol):

298.15-550 K: $\Delta Hf° = -92.159 - 6.607\times10^{-3}T + 2.410\times10^{-6}T^{2} - 532.200T^{-1}$
$\Delta Gf° = -92.159 + 6.607\times10^{-3}T\ln T - 2.410\times10^{-6}T^{2} - 266.100T^{-1} - 43.617\times10^{-3}T$
550-1134 K: $\Delta Hf° = -93.139 - 4.341\times10^{-3}T + 0.708\times10^{-6}T^{2} - 443.400T^{-1}$
$\Delta Gf° = -93.139 + 4.341\times10^{-3}T\ln T - 0.708\times10^{-6}T^{2} - 221.700T^{-1} - 28.620\times10^{-3}T$
1134-1193 K: $\Delta Hf° = -90.224 - 9.497\times10^{-3}T + 2.460\times10^{-6}T^{2} - 520.200T^{-1}$
$\Delta Gf° = -90.224 + 9.497\times10^{-3}T\ln T - 2.460\times10^{-6}T^{2} - 260.100T^{-1} - 65.440\times10^{-3}T$
1193-2000 K: $\Delta Hf° = -93.226 - 8.222\times10^{-3}T + 2.460\times10^{-6}T^{2} - 520.200T^{-1}$
$\Delta Gf° = -93.226 + 8.222\times10^{-3}T\ln T - 2.460\times10^{-6}T^{2} - 260.100T^{-1} - 53.891\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Topor (498). Low-temperature heat capacities and entropy at 298 K based on Westrum (526). Data above 1100 K based on Kapyrina (235). Data extrapolated from 298 to 1100 K.

$LaFeO_3(c)$
Lanthanum Ferrite
[Formation: $La(c) + Fe(c) + 1.5O_2(g) = LaFeO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	26.000	28.000	28.000	0	-333.000	-313.433	229.750
300	26.030	28.160	28.000	.050	-332.993	-313.309	228.243
400	27.540	35.860	29.035	2.730	-332.655	-306.800	167.626
500	28.880	42.150	31.030	5.560	-332.261	-300.369	131.289
550	29.515	44.934	32.174	7.018	-332.055	-297.191	118.091
550	29.515	44.934	32.174	7.018	-332.142	-297.191	118.091
600	30.150	47.530	33.347	8.510	-331.926	-294.024	107.097
700	31.390	52.270	35.727	11.580	-331.497	-287.743	89.836
800	32.610	56.550	38.075	14.780	-331.066	-281.535	76.911
900	33.830	60.460	40.338	18.110	-330.660	-275.359	66.866
1000	35.040	64.080	42.530	21.550	-330.369	-269.224	58.838

*Entropy and heat capacity at 298 K estimated.

Phase change: 550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 23.180 + 11.920\times10^{-3}T - 0.650\times10^{5}T^{-2}$

$H°-H°_{298} = 23.180\times10^{-3}T + 5.960\times10^{-6}T^{2} + 0.650\times10^{2}T^{-1} - 7.659$

Formation equations (kcal/mol):

298.15-550 K: $\Delta Hf° = -335.416 + 5.971\times10^{-3}T - 0.915\times10^{-6}T^{2} + 213.700T^{-1}$

$\Delta Gf° = -335.416 - 5.971\times10^{-3}T\ln T + 0.915\times10^{-6}T^{2} + 106.850T^{-1} + 106.275\times10^{-3}T$

550-1000 K: $\Delta Hf° = -336.396 + 8.237\times10^{-3}T - 2.617\times10^{-6}T^{2} + 302.500T^{-1}$

$\Delta Gf° = -336.396 - 8.237\times10^{-3}T\ln T + 2.617\times10^{-6}T^{2} + 151.250T^{-1} + 121.272\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Tret'yakov (502). Entropy and heat capacity at 298 K estimated. High-temperature data based on Kaul (237).

LaN(c)
Lanthanum Nitride
[Formation: La(c,l) + $0.5N_2$(g) = LaN(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	9.646	10.600	10.600	0	-72.500	-64.782	47.486
300	9.673	10.660	10.600	.018	-72.501	-64.735	47.158
400	10.679	13.598	10.993	1.042	-72.477	-62.149	33.956
500	11.233	16.045	11.767	2.139	-72.388	-59.574	26.040
550	11.421	17.126	12.206	2.706	-72.329	-58.296	23.164
550	11.421	17.126	12.206	2.706	-72.416	-58.296	23.164
600	11.609	18.128	12.658	3.282	-72.348	-57.015	20.768
700	11.902	19.940	13.571	4.458	-72.214	-54.466	17.005
800	12.150	21.546	14.470	5.661	-72.090	-51.944	14.190
900	12.371	22.990	15.338	6.887	-71.983	-49.433	12.004
1000	12.577	24.304	16.169	8.135	-71.896	-46.926	10.256
1100	12.772	25.512	16.964	9.403	-71.829	-44.431	8.827
1134	12.836	25.902	17.226	9.838	-71.811	-43.586	8.400
1134	12.836	25.902	17.226	9.838	-72.557	-43.586	8.400
1193	12.947	26.556	17.672	10.598	-72.592	-42.079	7.709
1193	12.947	26.556	17.672	10.598	-74.073	-42.079	7.709
1200	12.960	26.632	17.725	10.689	-74.068	-41.889	7.629
1300	13.143	27.676	18.450	11.994	-73.989	-39.218	6.593
1400	13.322	28.657	19.144	13.318	-73.895	-36.544	5.705
1500	13.498	29.582	19.809	14.659	-73.788	-33.873	4.935
1600	13.672	30.459	20.448	16.017	-73.669	-31.216	4.264
1700	13.845	31.293	21.062	17.393	-73.534	-28.578	3.674
1800	14.017	32.089	21.652	18.786	-73.385	-25.935	3.149

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 11.100 + 1.650 \times 10^{-3}T - 1.730 \times 10^{5}T^{-2}$
$H° - H°_{298} = 11.100 \times 10^{-3}T + 0.825 \times 10^{-6}T^{2} + 1.730 \times 10^{2}T^{-1} - 3.963$

Formation equations (kcal/mol):

298.15-550 K: $\Delta Hf° = -73.471 + 1.257 \times 10^{-3}T + 0.480 \times 10^{-6}T^{2} + 164.950T^{-1}$
$\Delta Gf° = -73.471 - 1.257 \times 10^{-3}T\ln T - 0.480 \times 10^{-6}T^{2} + 82.475T^{-1} + 35.515 \times 10^{-3}T$
550-1134 K: $\Delta Hf° = -74.450 + 3.523 \times 10^{-3}T - 1.222 \times 10^{-6}T^{2} + 253.750T^{-1}$
$\Delta Gf° = -74.450 - 3.523 \times 10^{-3}T\ln T + 1.222 \times 10^{-6}T^{2} + 126.875T^{-1} + 50.512 \times 10^{-3}T$
1134-1193 K: $\Delta Hf° = -71.535 - 1.633 \times 10^{-3}T + 0.530 \times 10^{-6}T^{2} + 176.950T^{-1}$
$\Delta Gf° = -71.535 + 1.633 \times 10^{-3}T\ln T - 0.530 \times 10^{-6}T^{2} + 88.475T^{-1} + 13.693 \times 10^{-3}T$
1193-1800 K: $\Delta Hf° = -74.537 - 0.358 \times 10^{-3}T + 0.530 \times 10^{-6}T^{2} + 176.950T^{-1}$
$\Delta Gf° = -74.537 + 0.358 \times 10^{-3}T\ln T - 0.530 \times 10^{-6}T^{2} + 88.475T^{-1} + 25.241 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (439). Other data are those estimated by Kubaschewski (289).

LaO(g)
Lanthanum Monoxide (ideal gas)
[Formation: La(c,l) + $0.5O_2(g)$ = LaO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.610	57.261	57.261	0	-29.000	-34.712	25.444
300	7.620	57.308	57.261	.014	-29.004	-34.748	25.313
400	8.000	59.558	57.565	.797	-29.228	-36.630	20.013
500	8.240	61.371	58.151	1.610	-29.438	-38.453	16.808
550	8.330	62.161	58.479	2.025	-29.540	-39.348	15.635
550	8.330	62.161	58.479	2.025	-29.627	-39.348	15.635
600	8.420	62.890	58.817	2.444	-29.727	-40.228	14.653
700	8.560	64.200	59.496	3.293	-29.946	-41.959	13.100
800	8.690	65.352	60.157	4.156	-30.190	-43.663	11.928
900	8.810	66.382	60.792	5.031	-30.462	-45.332	11.008
1000	8.920	67.316	61.399	5.917	-30.762	-46.963	10.264
1100	9.030	68.171	61.976	6.814	-31.092	-48.566	9.649
1134	9.064	68.446	62.166	7.122	-31.210	-49.106	9.464
1134	9.064	68.446	62.166	7.122	-31.956	-49.106	9.464
1193	9.123	68.908	62.488	7.658	-32.229	-49.991	9.158
1193	9.123	68.908	62.488	7.658	-33.710	-49.991	9.158
1200	9.130	68.961	62.526	7.722	-33.733	-50.085	9.122
1300	9.240	69.696	63.049	8.641	-34.062	-51.442	8.648
1400	9.350	70.385	63.549	9.570	-34.385	-52.764	8.237
1500	9.450	71.033	64.026	10.510	-34.700	-54.059	7.876
1600	9.560	71.647	64.484	11.461	-35.007	-55.339	7.559
1700	9.670	72.230	64.922	12.423	-35.306	-56.612	7.278
1800	9.780	72.786	65.344	13.396	-35.597	-57.854	7.024
1900	9.900	73.318	65.750	14.380	-35.880	-59.070	6.795
2000	10.010	73.828	66.141	15.375	-36.155	-60.285	6.587

Phase changes: 550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.983 + 0.998\times10^{-3}T - 0.597\times10^{5}T^{-2}$
$H°-H°_{298} = 7.983\times10^{-3}T + 0.499\times10^{-6}T^{2} + 0.597\times10^{2}T^{-1} - 2.625$

Formation equations (kcal/mol):

298.15-550 K: $\Delta Hf° = -28.441 - 2.217\times10^{-3}T + 0.198\times10^{-6}T^{2} + 25.100T^{-1}$
$\Delta Gf° = -28.441 + 2.217\times10^{-3}T\ln T - 0.198\times10^{-6}T^{2} + 12.550T^{-1} - 33.748\times10^{-3}T$
550-1134 K: $\Delta Hf° = -29.421 + 0.049\times10^{-3}T - 1.505\times10^{-6}T^{2} + 113.900T^{-1}$
$\Delta Gf° = -29.421 - 0.049\times10^{-3}T\ln T + 1.505\times10^{-6}T^{2} + 56.950T^{-1} - 18.751\times10^{-3}T$
1134-1193 K: $\Delta Hf° = -26.505 - 5.107\times10^{-3}T + 0.248\times10^{-6}T^{2} + 37.100T^{-1}$
$\Delta Gf° = -26.505 + 5.107\times10^{-3}T\ln T - 0.248\times10^{-6}T^{2} + 18.550T^{-1} - 55.570\times10^{-3}T$
1193-2000 K: $\Delta Hf° = -29.507 - 3.832\times10^{-3}T + 0.248\times10^{-6}T^{2} + 37.100T^{-1}$
$\Delta Gf° = -29.507 + 3.832\times10^{-3}T\ln T - 0.248\times10^{-6}T^{2} + 18.550T^{-1} - 44.022\times10^{-3}T$

Source: Data from Pedley (396).

$LaPO_4(c)$
Lanthanum Phosphate
[Formation: $La(c,l) + P(c,l,1/4P_4(g)) + 2O_2(g) = LaPO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	24.250	23.500	23.500	0	-455.000	-425.802	312.117
300	24.340	23.650	23.500	.045	-455.004	-425.621	310.061
317.3	24.970	25.032	23.546	.472	-455.032	-423.925	291.987
317.3	24.970	25.032	23.546	.472	-455.189	-423.925	291.987
400	27.980	31.210	24.507	2.681	-455.216	-415.772	227.164
500	30.120	37.700	26.514	5.593	-455.052	-405.924	177.427
550	30.890	40.609	27.661	7.121	-454.918	-401.029	159.352
550	30.890	40.609	27.661	7.121	-457.913	-401.029	159.352
600	31.660	43.330	28.855	8.685	-457.672	-395.868	144.193
700	32.920	48.310	31.287	11.916	-457.147	-385.605	120.390
800	34.040	52.780	33.699	15.265	-456.580	-375.429	102.561
900	35.070	56.850	36.049	18.721	-455.974	-365.322	88.711
1000	36.040	60.590	38.313	22.277	-455.330	-355.272	77.644
1100	36.980	64.070	40.499	25.928	-454.651	-345.298	68.603
1134	37.293	65.200	41.223	27.191	-454.411	-341.923	65.896
1134	37.293	65.200	41.223	27.191	-455.157	-341.923	65.896
1193	37.836	67.108	42.458	29.408	-454.790	-336.044	61.560
1193	37.836	67.108	42.458	29.408	-456.271	-336.044	61.560
1200	37.900	67.330	42.603	29.673	-456.216	-335.336	61.072
1300	38.800	70.400	44.625	33.507	-455.404	-325.307	54.688
1400	39.680	73.310	46.573	37.432	-454.518	-315.331	49.225
1500	40.560	76.080	48.451	41.444	-453.558	-305.421	44.499
1600	41.430	78.720	50.255	45.544	-452.524	-295.567	40.372

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.
550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 28.220 + 8.398\times10^{-3}T - 5.756\times10^{5}T^{-2}$
$H°-H°_{298} = 28.220\times10^{-3}T + 4.199\times10^{-6}T^{2} + 5.756\times10^{2}T^{-1} - 10.718$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -457.590 + 3.376\times10^{-3}T - 0.042\times10^{-6}T^{2} + 473.200T^{-1}$
$\Delta Gf° = -457.590 - 3.376\times10^{-3}T\ln T + 0.042\times10^{-6}T^{2} + 236.600T^{-1} + 123.178\times10^{-3}T$
317.3-550 K: $\Delta Hf° = -457.277 + 0.883\times10^{-3}T + 3.143\times10^{-6}T^{2} + 473.200T^{-1}$
$\Delta Gf° = -457.277 - 0.883\times10^{-3}T\ln T - 3.143\times10^{-6}T^{2} + 236.600T^{-1} + 108.842\times10^{-3}T$
550-1134 K: $\Delta Hf° = -461.717 + 4.487\times10^{-3}T + 1.437\times10^{-6}T^{2} + 461.700T^{-1}$
$\Delta Gf° = -461.717 - 4.487\times10^{-3}T\ln T - 1.437\times10^{-6}T^{2} + 230.850T^{-1} + 138.736\times10^{-3}T$
1134-1193 K: $\Delta Hf° = -458.801 - 0.669\times10^{-3}T + 3.189\times10^{-6}T^{2} + 384.900T^{-1}$
$\Delta Gf° = -458.801 + 0.669\times10^{-3}T\ln T - 3.189\times10^{-6}T^{2} + 192.450T^{-1} + 101.917\times10^{-3}T$
1193-1600 K: $\Delta Hf° = -461.803 + 0.606\times10^{-3}T + 3.189\times10^{-6}T^{2} + 384.900T^{-1}$
$\Delta Gf° = -461.803 - 0.606\times10^{-3}T\ln T - 3.189\times10^{-6}T^{2} + 192.450T^{-1} + 113.466\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Rat'kovskii (418). Other data based on Tsagareishvili (504).

La_2Se_3(c)
Dilanthanum Triselenide
[Reaction: $2La(c,l) + 1.5Se_2(g) = La_2Se_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	30.010	48.330	48.330	0	-272.950	-253.221	185.614
300*	30.040	48.520	48.320	.060	-272.941	-253.096	184.378
400	31.520	57.370	49.520	3.140	-272.658	-246.525	134.694
500	32.720	64.530	51.830	6.350	-272.273	-240.031	104.916
550	33.210	67.679	53.139	7.997	-272.045	-236.823	94.104
550	33.210	67.679	53.139	7.997	-272.219	-236.823	94.104
600	33.700	70.590	54.473	9.670	-271.962	-233.619	85.095
700	34.490	75.850	57.164	13.080	-271.423	-227.264	70.954
800	35.130	80.490	59.778	16.570	-270.861	-220.981	60.368
900	35.640	84.660	62.327	20.100	-270.317	-214.796	52.159
1000	36.060	88.440	64.750	23.690	-269.772	-208.647	45.599
1100	36.420	91.900	67.064	27.320	-269.247	-202.554	40.243
1134	36.522	93.010	67.825	28.560	-269.075	-200.498	38.640
1134	36.522	93.010	67.825	28.560	-270.567	-200.498	38.640
1193	36.699	94.865	69.121	30.713	-270.406	-196.862	36.063
1193	36.699	94.865	69.121	30.713	-273.368	-196.862	36.063
1200	36.720	95.080	69.272	30.970	-273.328	-196.408	35.770
1300	37.010	98.030	71.368	34.660	-272.753	-190.028	31.946
1400	37.310	100.780	73.366	38.380	-272.138	-183.679	28.673
1500	37.630	103.370	75.290	42.120	-271.495	-177.385	25.845

*Data above 298 K estimated.

Phase changes:
550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K:
$Cp° = 31.704 + 4.442\times10^{-3}T - 2.683\times10^{5}T^{-2}$
$H° - H°_{298} = 31.704\times10^{-3}T + 2.221\times10^{-6}T^{2} + 2.683\times10^{2}T^{-1} - 10.550$

Reaction equations (kcal/mol):

298.15-550 K:
$ΔHr° = -274.456 + 2.538\times10^{-3}T + 2.599\times10^{-6}T^{2} + 154.450T^{-1}$
$ΔGr° = -274.456 - 2.538\times10^{-3}T\ln T - 2.599\times10^{-6}T^{2} + 77.225T^{-1} + 85.587\times10^{-3}T$

550-1134 K:
$ΔHr° = -276.416 + 7.070\times10^{-3}T - 0.805\times10^{-6}T^{2} + 332.050T^{-1}$
$ΔGr° = -276.416 - 7.070\times10^{-3}T\ln T + 0.805\times10^{-6}T^{2} + 166.025T^{-1} + 115.582\times10^{-3}T$

1134-1193 K:
$ΔHr° = -270.584 - 3.242\times10^{-3}T + 2.700\times10^{-6}T^{2} + 178.450T^{-1}$
$ΔGr° = -270.584 + 3.242\times10^{-3}T\ln T - 2.700\times10^{-6}T^{2} + 89.225T^{-1} + 41.943\times10^{-3}T$

1193-1500 K:
$ΔHr° = -276.589 - 0.692\times10^{-3}T + 2.700\times10^{-6}T^{2} + 178.450T^{-1}$
$ΔGr° = -276.589 + 0.692\times10^{-3}T\ln T - 2.700\times10^{-6}T^{2} + 89.225T^{-1} + 65.041\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (332). Low-temperature heat capacities and entropy at 298 K from Paukov (394). Data above 298 K estimated.

$La_2Te_3(c)$
Dilanthanum Tritelluride
[Reaction: $2La(c,l) + 1.5Te_2(g) = La_2Te_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	31.580	55.360	55.360	0	-244.995	-225.721	165.456
300*	31.620	55.550	55.350	.060	-244.983	-225.600	164.347
400	33.300	64.900	56.625	3.310	-244.356	-219.238	119.784
500	34.430	72.460	59.060	6.700	-243.624	-213.036	93.117
550	34.845	75.760	60.419	8.437	-243.228	-209.983	83.438
550	34.845	75.760	60.419	8.437	-243.402	-209.983	83.438
600	35.260	78.810	61.827	10.190	-242.995	-206.965	75.386
700	35.930	84.300	64.657	13.750	-242.185	-201.021	62.761
800	36.490	89.140	67.427	17.370	-241.400	-195.212	53.329
900	36.970	93.460	70.082	21.040	-240.651	-189.486	46.013
1000	37.400	97.380	72.620	24.760	-239.944	-183.829	40.175
1100	37.770	100.960	75.033	28.520	-239.288	-178.237	35.412
1134	37.889	102.112	75.827	29.806	-239.077	-176.357	33.988
1134	37.889	102.112	75.827	29.806	-240.569	-176.357	33.988
1193	38.096	104.047	77.179	32.053	-240.337	-173.025	31.697
1193	38.096	104.047	77.179	32.053	-243.299	-173.025	31.697
1200	38.120	104.270	77.337	32.320	-243.253	-172.609	31.436
1300	38.420	107.330	79.530	36.140	-242.610	-166.768	28.036
1400	38.710	110.190	81.619	40.000	-241.952	-160.955	25.126
1500	38.970	112.870	83.617	43.880	-241.279	-155.187	22.610

*Data above 298 K estimated.

Phase changes: 550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 33.697 + 3.890\text{x}10^{-3}T - 2.913\text{x}10^{5}T^{-2}$
$H°- H°_{298} = 33.697\text{x}10^{-3}T + 1.945\text{x}10^{-6}T^{2} + 2.913\text{x}10^{2}T^{-1} - 11.197$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -248.129 + 7.628\text{x}10^{-3}T + 0.956\text{x}10^{-6}T^{2} + 231.000T^{-1}$
$\Delta Gr° = -248.129 - 7.628\text{x}10^{-3}T\ln T - 0.956\text{x}10^{-6}T^{2} + 115.500T^{-1} + 117.607\text{x}10^{-3}T$
550-1134 K: $\Delta Hr° = -250.089 + 12.160\text{x}10^{-3}T - 2.448\text{x}10^{-6}T^{2} + 408.600T^{-1}$
$\Delta Gr° = -250.089 - 12.160\text{x}10^{-3}T\ln T + 2.448\text{x}10^{-6}T^{2} + 204.300T^{-1} + 147.601\text{x}10^{-3}T$
1134-1193 K: $\Delta Hr° = -244.258 + 1.848\text{x}10^{-3}T + 1.056\text{x}10^{-6}T^{2} + 255.000T^{-1}$
$\Delta Gr° = -244.258 - 1.848\text{x}10^{-3}T\ln T - 1.056\text{x}10^{-6}T^{2} + 127.500T^{-1} + 73.962\text{x}10^{-3}T$
1193-1500 K: $\Delta Hr° = -250.262 + 4.398\text{x}10^{-3}T + 1.056\text{x}10^{-6}T^{2} + 255.000T^{-1}$
$\Delta Gr° = -250.262 - 4.398\text{x}10^{-3}T\ln T - 1.056\text{x}10^{-6}T^{2} + 127.500T^{-1} + 97.060\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (332). Low-temperature heat capacities and entropy at 298 K from Nogteva (355). Data above 298 K estimated.

$LiAlCl_4(c,l)$
Lithium Tetrachloroaluminate
[Formation: $Li(c,l) + Al(c,l) + 2Cl_2(g) = LiAlCl_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	35.400	25.900	25.900	0	-279.400	-251.252	184.170
300	35.400	26.120	25.920	.060	-279.392	-251.083	182.912
400	35.400	36.290	27.290	3.600	-278.731	-241.745	132.082
418	35.400	37.850	27.706	4.240	-278.626	-240.081	125.524
418	44.200	48.400	27.706	8.650	-274.216	-240.081	125.524
453.7	44.200	52.022	29.479	10.228	-273.712	-237.188	114.253
453.7	44.200	52.022	29.479	10.228	-274.429	-237.188	114.253
500	44.200	56.320	31.780	12.270	-273.809	-233.421	102.027
600	44.200	64.380	36.547	16.700	-272.481	-225.458	82.122
700	44.200	71.200	41.029	21.120	-271.199	-217.728	67.977
800	44.200	77.110	45.185	25.540	-269.962	-210.183	57.419
900	44.200	82.310	49.021	29.960	-268.773	-202.776	49.240
933.61	44.200	83.931	50.249	31.446	-268.385	-200.319	46.892
933.61	44.200	83.931	50.249	31.446	-270.965	-200.319	46.892
1000	44.200	86.970	52.580	34.390	-270.171	-195.317	42.686

Phase changes: 418 K, melting point of $LiALCl_4$; ΔH° = 4.410 kcal/mol.
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-418 K: $Cp^\circ = 35.380$
$H^\circ - H^\circ_{298} = 35.380\times10^{-3}T - 10.549$
418-1000 K: $Cp^\circ = 44.220$
$H^\circ - H^\circ_{298} = 44.220\times10^{-3}T - 9.834$

Formation equations (kcal/mol):

298.15-418 K: $\Delta Hf^\circ = -282.034 + 11.435\times10^{-3}T - 7.361\times10^{-6}T^2 - 36.200T^{-1}$
$\Delta Gf^\circ = -282.034 - 11.435\times10^{-3}T\ln T + 7.361\times10^{-6}T^2 - 18.100T^{-1} + 166.404\times10^{-3}T$
418-453.7 K: $\Delta Hf^\circ = -281.319 + 20.275\times10^{-3}T - 7.361\times10^{-6}T^2 - 36.200T^{-1}$
$\Delta Gf^\circ = -281.319 - 20.275\times10^{-3}T\ln T + 7.361\times10^{-6}T^2 - 18.100T^{-1} + 218.047\times10^{-3}T$
453.7-933.61 K: $\Delta Hf^\circ = -280.879 + 15.177\times10^{-3}T - 1.897\times10^{-6}T^2 - 21.900T^{-1}$
$\Delta Gf^\circ = -280.879 - 15.177\times10^{-3}T\ln T + 1.897\times10^{-6}T^2 - 10.950T^{-1} + 188.336\times10^{-3}T$
933.61-1000 K: $\Delta Hf^\circ = -282.147 + 12.179\times10^{-3}T - 0.170\times10^{-6}T^2 - 39.300T^{-1}$
$\Delta Gf^\circ = -282.147 - 12.179\times10^{-3}T\ln T + 0.170\times10^{-6}T^2 - 19.650T^{-1} + 170.813\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Weppner (523, 524). Other data based on Denielou (119).

LiAlF$_4$(g)
Lithium Tetrafluoroaluminate
[Formation: Li(c,l,g) + Al(c,l) + 2F$_2$(g) = LiAlF$_4$(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°$_{298}$)/T	H°- H°$_{298}$	ΔHf°	ΔGf°	
298.15	23.850	78.008	78.008	0	-444.200	-434.478	318.477
300	23.913	78.156	78.009	.044	-444.206	-434.419	316.470
400	26.532	85.427	78.982	2.578	-444.429	-431.118	235.549
453.7	27.377	88.835	79.949	4.032	-444.530	-429.327	206.806
453.7	27.377	88.835	79.949	4.032	-445.247	-429.327	206.806
500	28.105	91.531	80.899	5.316	-445.341	-427.695	186.943
600	29.091	96.749	83.116	8.180	-445.501	-424.149	154.494
700	29.740	101.285	85.395	11.123	-445.636	-420.580	131.309
800	30.186	105.287	87.636	14.121	-445.773	-416.993	113.916
900	30.504	108.862	89.800	17.156	-445.931	-413.385	100.382
933.61	30.582	109.982	90.506	18.183	-445.991	-412.169	96.484
933.61	30.582	109.982	90.506	18.183	-448.571	-412.169	96.484
1000	30.737	112.089	91.870	20.219	-448.668	-409.579	89.512
1100	30.913	115.027	93.843	23.302	-448.804	-405.662	80.597
1200	31.049	117.723	95.723	26.400	-448.935	-401.735	73.165
1300	31.156	120.212	97.511	29.511	-449.059	-397.795	66.875
1400	31.242	122.525	99.217	32.631	-449.183	-393.849	61.482
1500	31.312	124.682	100.843	35.758	-449.304	-389.894	56.807
1600	31.369	126.705	102.397	38.893	-449.421	-385.927	52.714
1638	31.387	127.442	102.969	40.085	-449.465	-384.419	51.290
1638	31.387	127.442	102.969	40.085	-484.625	-384.419	51.290
1700	31.417	128.608	103.883	42.032	-484.585	-380.623	48.932
1800	31.457	130.405	105.307	45.176	-484.521	-374.510	45.471
1900	31.491	132.107	106.674	48.323	-484.457	-368.399	42.375
2000	31.520	133.723	107.986	51.474	-484.397	-362.293	39.589

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 30.155 + 0.952\times10^{-3}T - 5.857\times10^{5}T^{-2}$
$H° - H°_{298} = 30.155\times10^{-3}T + 0.476\times10^{-6}T^{2} + 5.857\times10^{2}T^{-1} - 10.997$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -447.241 + 6.848\times10^{-3}T - 7.057\times10^{-6}T^{2} + 485.100T^{-1}$
$\Delta Gf° = -447.241 - 6.848\times10^{-3}T\ln T + 7.057\times10^{-6}T^{2} + 242.550T^{-1} + 76.994\times10^{-3}T$
453.7-933.61 K: $\Delta Hf° = -446.802 + 1.750\times10^{-3}T - 1.593\times10^{-6}T^{2} + 499.400T^{-1}$
$\Delta Gf° = -446.802 - 1.750\times10^{-3}T\ln T + 1.593\times10^{-6}T^{2} + 249.700T^{-1} + 47.282\times10^{-3}T$
933.61-1638 K: $\Delta Hf° = -448.069 - 1.248\times10^{-3}T + 0.134\times10^{-6}T^{2} + 482.000T^{-1}$
$\Delta Gf° = -448.069 + 1.248\times10^{-3}T\ln T - 0.134\times10^{-6}T^{2} + 241.000T^{-1} + 29.759\times10^{-3}T$
1638-2000 K: $\Delta Hf° = -485.536 + 0.338\times10^{-3}T + 0.150\times10^{-6}T^{2} - 65.900T^{-1}$
$\Delta Gf° = -485.536 - 0.338\times10^{-3}T\ln T - 0.150\times10^{-6}T^{2} - 32.950T^{-1} + 64.499\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Dewing (121). Other data from JANAF (131) who estimated some molecular constants.

$Li_3AlF_6(c,l)$
Trilithium Hexafluoroaluminate
[Formation: $3Li(c,l) + Al(c,l) + 3F_2(g) = Li_3AlF_6(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	48.400	44.907	44.907	0	-804.900	-766.719	562.013
300	48.550	45.207	44.907	.090	-804.896	-766.483	558.376
400	54.940	60.122	46.900	5.289	-804.465	-753.733	411.815
453.7	57.281	67.210	48.887	8.313	-804.155	-746.947	359.804
453.7	57.281	67.210	48.887	8.313	-806.306	-746.947	359.804
500	59.300	72.874	50.850	11.012	-806.032	-740.896	323.841
600	62.690	83.996	55.466	17.118	-805.206	-727.940	265.148
700	65.500	93.876	60.260	23.531	-804.119	-715.147	223.276
748	66.700	98.263	62.560	26.706	-803.518	-709.066	207.171
748	66.700	98.931	62.560	27.206	-803.018	-709.066	207.171
800	68.000	103.457	65.072	30.708	-802.323	-702.561	191.928
848	69.200	107.453	67.358	34.001	-801.636	-696.594	179.527
848	69.200	107.807	67.358	34.301	-801.336	-696.594	179.527
900	70.500	111.964	69.816	37.933	-800.544	-690.192	167.599
933.61	71.340	114.564	71.381	40.317	-800.006	-686.081	160.603
933.61	71.340	114.564	71.381	40.317	-802.586	-686.081	160.603
978	72.450	117.903	73.416	43.508	-801.825	-680.562	152.081
978	72.450	118.005	73.416	43.608	-801.725	-680.562	152.081
1000	73.000	119.624	74.416	45.208	-801.329	-677.842	148.140
1058	74.450	123.780	77.009	49.484	-800.230	-670.708	138.546
1058	86.000	143.251	77.009	70.084	-779.630	-670.708	138.546
1100	86.000	146.599	79.603	73.696	-778.322	-666.410	132.402
1200	86.000	154.082	85.502	82.296	-775.218	-656.376	119.541
1300	86.000	160.966	91.046	90.896	-772.120	-646.597	108.701
1400	86.000	167.339	96.270	99.496	-769.034	-637.059	99.448
1500	86.000	173.272	101.208	108.096	-765.951	-627.741	91.461

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
748 K, α - β transition point of Li_3AlF_6; ΔH° = 0.500 kcal/mol.
848 K, β - γ transition point of Li_3AlF_6; ΔH° = 0.300 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
978 K, γ - δ transition point of Li_3AlF_6; ΔH° = 0.100 kcal/mol.
1058 K, melting point of Li_3AlF_6; ΔH° = 20.600 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-748 K: $Cp° = 51.048 + 23.190\times10^{-3}T - 8.500\times10^{5}T^{-2}$
$H°-H°_{298} = 51.048\times10^{-3}T + 11.595\times10^{-6}T^2 + 8.500\times10^{2}T^{-1} - 19.102$
748-848 K: $Cp° = 48.000 + 25.000\times10^{-3}T$
$H°-H°_{298} = 48.000\times10^{-3}T + 12.500\times10^{-6}T^2 - 15.692$
848-978 K: $Cp° = 48.000 + 25.000\times10^{-3}T$
$H°-H°_{298} = 48.000\times10^{-3}T + 12.500\times10^{-6}T^2 - 15.392$
978-1058 K: $Cp° = 48.000 + 25.000\times10^{-3}T$
$H°-H°_{298} = 48.000\times10^{-3}T + 12.500\times10^{-6}T^2 - 15.292$
1058-1500 K: $Cp° = 86.000$
$H°-H°_{298} = 86.000\times10^{-3}T - 20.904$

Formation equations (kcal/mol):

298.15-453.7 K: $ΔHf° = -811.730 + 15.835\times10^{-3}T - 7.028\times10^{-6}T^2 + 814.900T^{-1}$
$ΔGf° = -811.730 - 15.835\times10^{-3}T\ln T + 7.028\times10^{-6}T^2 + 407.450T^{-1} + 234.509\times10^{-3}T$
453.7-748 K: $ΔHf° = -810.410 + 0.541\times10^{-3}T + 9.364\times10^{-6}T^2 + 857.800T^{-1}$
$ΔGf° = -810.410 - 0.541\times10^{-3}T\ln T - 9.364\times10^{-6}T^2 + 428.900T^{-1} + 145.374\times10^{-3}T$
748-848 K: $ΔHf° = -807.001 - 2.507\times10^{-3}T + 10.269\times10^{-6}T^2 + 7.800T^{-1}$
$ΔGf° = -807.001 + 2.507\times10^{-3}T\ln T - 10.269\times10^{-6}T^2 + 3.900T^{-1} + 122.082\times10^{-3}T$
848-933.61 K: $ΔHf° = -806.701 - 2.507\times10^{-3}T + 10.269\times10^{-6}T^2 + 7.800T^{-1}$
$ΔGf° = -806.701 + 2.507\times10^{-3}T\ln T - 10.269\times10^{-6}T^2 + 3.900T^{-1} + 121.729\times10^{-3}T$
933.61-978 K: $ΔHf° = -807.968 - 5.505\times10^{-3}T + 11.996\times10^{-6}T^2 - 9.600T^{-1}$
$ΔGf° = -807.968 + 5.505\times10^{-3}T\ln T - 11.996\times10^{-6}T^2 - 4.800T^{-1} + 104.205\times10^{-3}T$
978-1058 K: $ΔHf° = -807.868 - 5.505\times10^{-3}T + 11.996\times10^{-6}T^2 - 9.600T^{-1}$
$ΔGf° = -807.868 + 5.505\times10^{-3}T\ln T - 11.996\times10^{-6}T^2 - 4.800T^{-1} + 104.103\times10^{-3}T$
1058-1500 K: $ΔHf° = -813.480 + 32.495\times10^{-3}T - 0.504\times10^{-6}T^2 - 9.600T^{-1}$
$ΔGf° = -813.480 - 32.495\times10^{-3}T\ln T + 0.504\times10^{-6}T^2 - 4.800T^{-1} + 360.820\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127).

$LiAlO_2(c)$
Lithium Aluminate
Formation: $Li(c,l,g) + Al(c,l) + O_2(g) = LiAlO_2(c)]$

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	16.200	12.750	12.750	0	-285.210	-270.307	198.138
300	16.287	12.850	12.750	.030	-285.215	-270.215	196.849
400	19.430	18.023	13.433	1.836	-285.338	-265.190	144.891
453.7	20.307	20.541	14.126	2.910	-285.351	-262.485	126.439
453.7	20.307	20.541	14.126	2.910	-286.068	-262.485	126.439
500	21.064	22.551	14.815	3.868	-286.079	-260.075	113.677
600	22.099	26.488	16.440	6.029	-286.037	-254.876	92.837
700	22.851	29.954	18.128	8.278	-285.948	-249.690	77.956
800	23.450	33.046	19.804	10.594	-285.841	-244.519	66.799
900	23.959	35.838	21.432	12.965	-285.735	-239.361	58.124
933.61	24.111	36.719	21.967	13.773	-285.701	-237.630	55.626
933.61	24.111	36.719	21.967	13.773	-288.281	-237.630	55.626
1000	24.412	38.386	23.002	15.384	-288.183	-234.031	51.147
1100	24.827	40.732	24.508	17.846	-288.007	-228.623	45.423
1200	25.216	42.909	25.951	20.349	-287.799	-223.233	40.656
1300	25.586	44.942	27.335	22.889	-287.560	-217.863	36.626
1400	25.942	46.852	28.663	25.465	-287.292	-212.512	33.174
1500	26.286	48.653	29.935	28.077	-286.992	-207.182	30.186
1600	26.621	50.360	31.159	30.722	-286.664	-201.870	27.574
1638	26.745	50.986	31.611	31.736	-286.531	-199.859	26.666
1638	26.745	50.986	31.611	31.736	-321.691	-199.859	26.666
1700	26.948	51.984	32.336	33.401	-321.354	-195.251	25.101
1800	27.269	53.534	33.472	36.112	-320.787	-187.850	22.808
1900	27.585	55.016	34.567	38.854	-320.196	-180.479	20.760
2000	27.896	56.439	35.625	41.628	-319.578	-173.142	18.920

Phase changes:
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1638 K, boiling poing of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.
1973 K, melting point of $LiAlO_2$; ΔH° = 21 ± 5 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.854 + 3.126\times10^{-3}T - 5.855\times10^{5}T^{-2}$
$H°-H°_{298} = 21.854\times10^{-3}T + 1.563\times10^{-6}T^{2} + 5.855\times10^{2}T^{-1} - 8.618$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -289.299 + 8.333\times10^{-3}T - 6.125\times10^{-6}T^{2} + 640.700T^{-1}$
$\Delta Gf° = -289.299 - 8.333\times10^{-3}T\ln T + 6.125\times10^{-6}T^{2} + 320.350T^{-1} + 105.748\times10^{-3}T$
453.7-933.61 K: $\Delta Hf° = -288.859 + 3.235\times10^{-3}T - 0.661\times10^{-6}T^{2} + 655.000T^{-1}$
$\Delta Gf° = -288.859 - 3.235\times10^{-3}T\ln T + 0.661\times10^{-6}T^{2} + 327.500T^{-1} + 76.036\times10^{-3}T$
933.61-1638 K: $\Delta Hf° = -290.127 + 0.237\times10^{-3}T + 1.066\times10^{-6}T^{2} + 637.600T^{-1}$
$\Delta Gf° = -290.127 - 0.237\times10^{-3}T\ln T - 1.066\times10^{-6}T^{2} + 318.800T^{-1} + 58.513\times10^{-3}T$
1638-2000 K: $\Delta Hf° = -327.593 + 1.823\times10^{-3}T + 1.082\times10^{-6}T^{2} + 89.700T^{-1}$
$\Delta Gf° = -327.593 - 1.823\times10^{-3}T\ln T - 1.082\times10^{-6}T^{2} + 44.850T^{-1} + 93.253\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from King (260). High-temperature data based on Christensen (93). Enthalpy of fusion estimated by JANAF (131).

$LiAlSiO_4(\beta)$
Lithium Aluminum Silicate, β-Eucryptite
[Formation: $Li(c,l) + Al(c,l) + Si(c) + 2O_2(g) = LiAlSiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ-H^\circ_{298})/T$	$H^\circ-H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	27.090	24.810	24.810	0	-505.045	-477.785	350.221
300	27.191	24.978	24.811	.050	-505.052	-477.616	347.939
400	31.938	33.475	25.937	3.015	-505.233	-468.437	255.939
453.7	33.904	37.636	27.076	4.791	-505.223	-463.497	223.266
453.7	33.904	37.636	27.076	4.791	-505.940	-463.497	223.266
500	35.599	41.013	28.213	6.400	-505.898	-459.165	200.698
600	38.359	47.760	30.918	10.105	-505.639	-449.839	163.852
700	40.367	53.833	33.766	14.047	-505.226	-440.571	137.551
800	41.752	59.320	36.623	18.158	-504.727	-431.369	117.843
900	42.632	64.293	39.425	22.381	-504.203	-422.230	102.530
933.61	42.796	65.859	40.349	23.817	-504.028	-419.172	98.123
933.61	42.796	65.859	40.349	23.817	-506.608	-419.172	98.123
1000	43.121	68.813	42.142	26.671	-506.235	-412.960	90.251
1100	43.332	72.934	44.756	30.996	-505.672	-403.666	80.200
1200	43.379	76.708	47.265	35.332	-505.123	-394.418	71.832
1300	43.380	80.179	49.664	39.670	-504.592	-385.215	64.760
1300	46.600	80.410	49.664	39.970	-504.292	-385.215	64.760
1400	47.800	83.908	51.987	44.690	-503.401	-376.084	58.709
1500	49.000	87.246	54.226	49.530	-502.406	-367.036	53.476
1600	50.200	90.447	56.391	54.490	-501.308	-358.047	48.906

Phase changes: 453.7 K, melting point of Li; $\Delta H^\circ = 0.717$ kcal/mol.
933.61 K, melting point of Al; $\Delta H^\circ = 2.580$ kcal/mol.
1300 K, α - β transition point of $LiAlSiO_4$; $\Delta H^\circ = 0.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $C_p^\circ = 36.739 + 6.940\times10^{-3}T - 10.416\times10^{5}T^{-2}$
$H^\circ-H^\circ_{298} = 36.739\times10^{-3}T + 3.470\times10^{-6}T^2 + 10.416\times10^{2}T^{-1} - 14.756$
1300-1600 K: $C_p^\circ = 31.000 + 12.000\times10^{-3}T$
$H^\circ-H^\circ_{298} = 31.000\times10^{-3}T + 6.000\times10^{-6}T^2 - 10.470$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -510.865 + 10.309\times10^{-3}T - 5.072\times10^{-6}T^2 + 953.100T^{-1}$
$\Delta Gf^\circ = -510.865 - 10.309\times10^{-3}T\ln T + 5.072\times10^{-6}T^2 + 476.550T^{-1} + 162.812\times10^{-3}T$
453.7-933.61 K: $\Delta Hf^\circ = -510.425 + 5.211\times10^{-3}T + 0.392\times10^{-6}T^2 + 967.400T^{-1}$
$\Delta Gf^\circ = -510.425 - 5.211\times10^{-3}T\ln T - 0.392\times10^{-6}T^2 + 483.700T^{-1} + 133.100\times10^{-3}T$
933.61-1300 K: $\Delta Hf^\circ = -511.692 + 2.213\times10^{-3}T + 2.119\times10^{-6}T^2 + 950.000T^{-1}$
$\Delta Gf^\circ = -511.692 - 2.213\times10^{-3}T\ln T - 2.119\times10^{-6}T^2 + 475.000T^{-1} + 115.577\times10^{-3}T$
1300-1600 K: $\Delta Hf^\circ = -507.406 - 3.526\times10^{-3}T + 4.649\times10^{-6}T^2 - 91.600T^{-1}$
$\Delta Gf^\circ = -507.406 + 3.526\times10^{-3}T\ln T - 4.649\times10^{-6}T^2 - 45.800T^{-1} + 74.728\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Barany (20). Other data based on Pankratz (390).

$LiAlSi_2O_6(\alpha)$

Lithium Aluminum Disilicate, α-Spodumene

[Formation: $Li(c,l) + Al(c,l) + 2Si(c) + 3O_2(g) = LiAlSi_2O_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^\circ_{298})/T$	$H°-H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	37.980	30.860	30.860	0	-727.725	-686.316	503.077
300	38.128	31.095	30.862	.070	-727.734	-686.060	499.788
400	44.266	42.963	32.436	4.211	-727.956	-672.128	367.229
453.7	46.548	48.702	34.025	6.659	-727.953	-664.630	320.152
453.7	46.548	48.702	34.025	6.659	-728.670	-664.630	320.152
500	48.515	53.321	35.601	8.860	-728.634	-658.094	287.649
600	51.773	62.466	39.331	13.881	-728.386	-644.007	234.577
700	54.376	70.649	43.230	19.193	-727.972	-629.976	196.685
800	56.464	78.052	47.128	24.739	-727.441	-616.012	168.285
900	58.103	84.801	50.944	30.471	-726.842	-602.118	146.212
933.61	58.515	86.939	52.202	32.431	-726.630	-597.464	139.859
933.61	58.515	86.939	52.202	32.431	-729.210	-597.464	139.859
1000	59.330	90.990	54.644	36.346	-728.744	-588.096	128.527
1100	60.164	96.687	58.211	42.324	-728.004	-574.081	114.058
1150	60.437	99.368	59.943	45.339	-727.624	-567.094	107.771

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1150 K: $Cp° = 44.428 + 16.340\times10^{-3}T - 10.063\times10^{5}T^{-2}$

$H°-H^\circ_{298} = 44.428\times10^{-3}T + 8.170\times10^{-6}T^2 + 10.063\times10^{2}T^{-1} - 17.348$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -731.730 + 5.089\times10^{-3}T - 1.226\times10^{-6}T^2 + 774.100T^{-1}$

$\Delta Gf° = -731.730 - 5.089\times10^{-3}T\ln T + 1.226\times10^{-6}T^2 + 387.050T^{-1} + 176.592\times10^{-3}T$

453.7-933.61 K: $\Delta Hf° = -731.290 - 0.009\times10^{-3}T + 4.238\times10^{-6}T^2 + 788.400T^{-1}$

$\Delta Gf° = -731.290 + 0.009\times10^{-3}T\ln T - 4.238\times10^{-6}T^2 + 394.200T^{-1} + 146.880\times10^{-3}T$

933.61-1150 K: $\Delta Hf° = -732.558 - 3.007\times10^{-3}T + 5.965\times10^{-6}T^2 + 771.000T^{-1}$

$\Delta Gf° = -732.558 + 3.007\times10^{-3}T\ln T - 5.965\times10^{-6}T^2 + 385.500T^{-1} + 129.357\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Barany (20). Other data based on Pankratz (390).

$LiAlSi_2O_6(\beta)$
Lithium Aluminum Disilicate, β-Spodumene
[Formation: $Li(c,l) + Al(c,l) + 2Si(c,l) + 3O_2(g) = LiAlSi_2O_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	38.900	36.890	36.890	0	-720.985	-681.374	499.454
300	39.057	37.131	36.891	.072	-720.992	-681.129	496.195
400	45.638	49.370	38.515	4.342	-721.085	-667.819	364.875
453.7	47.870	55.284	40.153	6.865	-721.007	-660.671	318.245
453.7	47.870	55.284	40.153	6.865	-721.724	-660.671	318.245
500	49.794	60.029	41.777	9.126	-721.628	-654.442	286.053
600	52.801	69.386	45.614	14.263	-721.264	-641.037	233.495
700	55.094	77.705	49.615	19.663	-720.762	-627.705	195.976
800	56.898	85.184	53.601	25.266	-720.174	-614.451	167.858
900	58.351	91.973	57.495	31.030	-719.543	-601.274	146.007
933.61	58.758	94.120	58.775	32.998	-719.322	-596.861	139.718
933.61	58.758	94.120	58.775	32.998	-721.902	-596.861	139.718
1000	59.562	98.185	61.257	36.928	-721.422	-587.969	128.499
1100	60.618	103.912	64.877	42.938	-720.650	-574.675	114.176
1200	61.602	109.229	68.355	49.049	-719.818	-561.441	102.251
1300	62.588	114.198	71.692	55.258	-718.922	-548.280	92.173
1400	63.650	118.875	74.897	61.569	-717.961	-535.181	83.544
1500	64.859	123.306	77.977	67.993	-716.915	-522.185	76.081
1600	66.285	127.537	80.945	74.548	-715.767	-509.244	69.559
1638	66.936	129.101	82.044	77.079	-715.297	-504.345	67.291
1638	66.936	129.101	82.044	77.079	-750.457	-504.345	67.291
1687	67.775	131.084	83.439	80.377	-749.734	-496.947	64.378
1687	67.775	131.084	83.439	80.377	-773.898	-496.947	64.378
1700	67.998	131.605	83.805	81.260	-773.682	-494.805	63.611

Phase changes:
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1700 K:
$Cp° = 49.541 + 10.892\times10^{-3}T - 12.346\times10^{5}T^{-2}$
$H°-H°_{298} = 49.541\times10^{-3}T + 5.446\times10^{-6}T^{2} + 12.346\times10^{2}T^{-1} - 19.396$

Formation equations (kcal/mol):

298.15-453.7 K:
$\Delta Hf° = -727.038 + 10.202\times10^{-3}T - 3.950\times10^{-6}T^{2} + 1002.400T^{-1}$
$\Delta Gf° = -727.038 - 10.202\times10^{-3}T\ln T + 3.950\times10^{-6}T^{2} + 501.200T^{-1} + 204.467\times10^{-3}T$

453.7-933.61 K:
$\Delta Hf° = -726.598 + 5.104\times10^{-3}T + 1.514\times10^{-6}T^{2} + 1016.700T^{-1}$
$\Delta Gf° = -726.598 - 5.104\times10^{-3}T\ln T - 1.514\times10^{-6}T^{2} + 508.350T^{-1} + 174.755\times10^{-3}T$

933.61-1638 K:
$\Delta Hf° = -727.866 + 2.106\times10^{-3}T + 3.241\times10^{-6}T^{2} + 999.300T^{-1}$
$\Delta Gf° = -727.866 - 2.106\times10^{-3}T\ln T - 3.241\times10^{-6}T^{2} + 499.650T^{-1} + 157.232\times10^{-3}T$

1638-1687 K:
$\Delta Hf° = -765.332 + 3.692\times10^{-3}T + 3.257\times10^{-6}T^{2} + 451.400T^{-1}$
$\Delta Gf° = -765.332 - 3.692\times10^{-3}T\ln T - 3.257\times10^{-6}T^{2} + 225.700T^{-1} + 191.972\times10^{-3}T$

1687-1700 K:
$\Delta Hf° = -790.190 + 2.850\times10^{-3}T + 3.959\times10^{-6}T^{2} + 648.400T^{-1}$
$\Delta Gf° = -790.190 - 2.850\times10^{-3}T\ln T - 3.959\times10^{-6}T^{2} + 324.200T^{-1} + 201.600\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Barany (20). Other data based on Pankratz (390).

$Li_2Al_2Si_8O_{20}(c)$
Lithium Aluminum Silicate, Petalite
[Formation: $2Li(c,l) + 2Al(c,l) + 8Si(c) + 10O_2(g) = Li_2Al_2Si_8O_{20}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	117.200	111.000	111.000	0	-2335.800	-2203.866	1615.456
300	117.600	111.700	111.000	.220	-2335.826	-2203.036	1604.890
400	139.700	148.900	115.950	13.180	-2336.460	-2158.681	1179.433
453.7	147.701	167.012	120.855	20.942	-2336.304	-2134.774	1028.319
453.7	147.701	167.012	120.855	20.942	-2337.738	-2134.774	1028.319
500	154.600	181.700	125.820	27.940	-2337.462	-2114.070	924.047
600	165.300	210.900	137.633	43.960	-2336.296	-2069.511	753.809
700	173.000	237.000	150.000	60.900	-2334.628	-2025.179	632.281
800	178.400	260.500	162.400	78.480	-2332.690	-1981.125	541.211
900	182.300	281.700	174.444	96.530	-2330.642	-1937.250	470.423
933.61	183.241	288.401	178.427	102.673	-2329.942	-1922.572	450.051
933.61	183.241	288.401	178.427	102.673	-2335.102	-1922.572	450.051
1000	185.100	301.100	186.200	114.900	-2333.646	-1893.270	413.769
1100	187.400	318.800	197.436	133.500	-2331.426	-1849.369	367.431
1200	189.700	335.200	208.200	152.400	-2329.052	-1805.598	328.840
1250	191.000	343.000	213.480	161.900	-2327.860	-1783.872	311.888

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1250 K: $Cp° = 147.100 + 44.382\times10^{-3}T - 38.409\times10^{5}T^{-2}$
$H°-H°_{298} = 147.100\times10^{-3}T + 22.191\times10^{-6}T^2 + 38.409\times10^{2}T^{-1} - 58.713$

Formation equations (kcal/mol):

298.15-453.7 K: $ΔHf° = -2350.200 + 16.786\times10^{-3}T - 0.017\times10^{-6}T^2 + 2801.700T^{-1}$
$ΔGf° = -2350.200 - 16.786\times10^{-3}T\ln T + 0.017\times10^{-6}T^2 + 1400.850T^{-1} + 570.684\times10^{-3}T$
453.7-933.61 K: $ΔHf° = -2349.321 + 6.590\times10^{-3}T + 10.911\times10^{-6}T^2 + 2830.300T^{-1}$
$ΔGf° = -2349.321 - 6.590\times10^{-3}T\ln T - 10.911\times10^{-6}T^2 + 1415.150T^{-1} + 511.261\times10^{-3}T$
933.61-1250 K: $ΔHf° = -2351.856 + 0.594\times10^{-3}T + 14.365\times10^{-6}T^2 + 2795.500T^{-1}$
$ΔGf° = -2351.856 - 0.594\times10^{-3}T\ln T - 14.365\times10^{-6}T^2 + 1397.750T^{-1} + 476.215\times10^{-3}T$

Source: Data from Bennington (36).

$LiBF_4(c,l)$
Lithium Tetrafluoroborate
[Formation: $Li(c,l) + B(\beta) + 2F_2(g) = LiBF_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	26.800	32.200	32.200	0	-440.600	-418.820	306.999
300	26.830	32.366	32.200	.050	-440.594	-418.684	305.007
400	29.110	40.410	33.285	2.850	-440.270	-411.432	224.793
453.7	30.136	44.144	34.348	4.444	-440.108	-407.570	196.326
453.7	30.136	44.144	34.348	4.444	-440.825	-407.570	196.326
500	31.020	47.115	35.395	5.860	-440.693	-404.180	176.665
583	32.480	51.989	37.418	8.495	-440.417	-398.144	149.251
583	40.100	57.821	37.418	11.895	-437.017	-398.144	149.251
600	40.100	58.973	38.015	12.575	-436.826	-397.014	144.610
700	40.100	65.155	41.462	16.585	-435.730	-390.466	121.907

*Heat capacity at 298 K estimated.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
583 K, melting point of $LiBF_4$; ΔH° = 3.400 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-583 K: $Cp^\circ = 23.629 + 15.902\text{x}10^{-3}T - 1.412\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 23.629\text{x}10^{-3}T + 7.951\text{x}10^{-6}T^{2} + 1.412\text{x}10^{2}T^{-1} - 8.225$
553-700 K: $Cp^\circ = 40.100$
$H^\circ - H^\circ_{298} = 40.100\text{x}10^{-3}T - 11.483$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -440.121 + 0.191\text{x}10^{-3}T + 1.453\text{x}10^{-6}T^{2} - 198.300T^{-1}$
$\Delta Gf^\circ = -440.121 - 0.191\text{x}10^{-3}T\ln T - 1.453\text{x}10^{-6}T^{2} - 99.150T^{-1} + 74.080\text{x}10^{-3}T$
453.7-583 K: $\Delta Hf^\circ = -439.681 - 4.907\text{x}10^{-3}T + 6.917\text{x}10^{-6}T^{2} - 184.000T^{-1}$
$\Delta Gf^\circ = -439.681 + 4.907\text{x}10^{-3}T\ln T - 6.917\text{x}10^{-6}T^{2} - 92.000T^{-1} + 44.369\text{x}10^{-3}T$
583-700 K: $\Delta Hf^\circ = -442.939 + 11.564\text{x}10^{-3}T - 1.034\text{x}10^{-6}T^{2} - 325.200T^{-1}$
$\Delta Gf^\circ = -442.939 - 11.564\text{x}10^{-3}T\ln T + 1.034\text{x}10^{-6}T^{2} - 162.600T^{-1} + 150.420\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Entropy at 298 K based on Plakhotnik (404). Heat capacity at 298 K estimated. High-temperature data based on Dworkin (132).

$LiBH_4$(c)
Lithium Borohydride
[Formation: $Li(c,l) + B(\beta) + 2H_2(g) = LiBH_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.727	18.120	18.120	0	-45.522	-29.822	21.860
300*	19.835	18.242	18.120	.037	-45.527	-29.724	21.653
400	21.750	24.231	18.924	2.123	-45.767	-24.420	13.342
453.7	22.684	27.030	19.721	3.316	-45.901	-21.547	10.379
453.7	22.684	27.030	19.721	3.316	-46.618	-21.547	10.379
500	23.490	29.273	20.503	4.385	-46.728	-18.981	8.296
600	25.130	33.708	22.340	6.821	-46.880	-13.417	4.887
700	26.270	37.672	24.252	9.394	-46.929	-7.834	2.446
800	27.020	41.234	26.157	12.062	-46.911	-2.249	.614

*Data above 298 K estimated.

Phase change: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp^\circ = 18.482 + 11.620\text{x}10^{-3}T - 1.973\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.482\text{x}10^{-3}T + 5.810\text{x}10^{-6}T^2 + 1.973\text{x}10^{2}T^{-1} - 6.689$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -45.471 - 0.852\text{x}10^{-3}T - 1.178\text{x}10^{-6}T^2 + 91.800T^{-1}$

$\Delta Gf^\circ = -45.471 + 0.852\text{x}10^{-3}T\ln T + 1.178\text{x}10^{-6}T^2 + 45.900T^{-1} + 46.766\text{x}10^{-3}T$

453.7-800 K: $\Delta Hf^\circ = -45.031 - 5.950\text{x}10^{-3}T + 4.286\text{x}10^{-6}T^2 + 106.100T^{-1}$

$\Delta Gf^\circ = -45.031 + 5.950\text{x}10^{-3}T\ln T - 4.286\text{x}10^{-6}T^2 + 53.050T^{-1} + 17.054\text{x}10^{-3}T$

Source: Data from JANAF (127) who estimated all above 298 K.

$LiBO_2$(c,l,g)
Lithium Borate
[Formation: Li(c,l,g) + B(β) + O_2(g) = $LiBO_2$(c,l,g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	14.429	12.364	12.364	0	-243.600	-230.182	168.726
300	14.488	12.453	12.364	.027	-243.602	-230.097	167.624
400	17.004	16.996	12.966	1.612	-243.665	-225.586	123.253
453.7	17.961	19.204	13.576	2.553	-243.689	-223.157	107.495
453.7	17.961	19.204	13.576	2.553	-244.406	-223.157	107.495
500	18.787	20.989	14.181	3.404	-244.429	-220.986	96.591
600	20.329	24.553	15.618	5.361	-244.415	-216.299	78.786
700	21.773	27.796	17.129	7.467	-244.305	-211.619	66.070
800	23.169	30.795	18.653	9.714	-244.094	-206.964	56.539
900	24.540	33.603	20.159	12.100	-243.782	-202.339	49.134
1000	25.897	36.259	21.637	14.622	-243.365	-197.755	43.219
1100	27.244	38.790	23.082	17.279	-242.839	-193.224	38.389
1117	27.472	39.210	23.325	17.744	-242.739	-192.458	37.655
1117	34.491	46.444	23.325	25.824	-234.659	-192.458	37.655
1200	34.491	48.916	25.010	28.687	-233.586	-189.360	34.487
1300	34.491	51.677	26.956	32.137	-232.312	-185.723	31.222
1400	34.491	54.233	28.814	35.586	-231.060	-182.186	28.440
1500	34.491	56.612	30.589	39.035	-229.827	-178.734	26.041
1600	34.491	58.838	32.286	42.484	-228.614	-175.379	23.955
1638	34.491	59.648	32.911	43.795	-228.157	-174.120	23.232
1638	34.491	59.648	32.911	43.795	-263.317	-174.120	23.232
1700	34.491	60.929	33.910	45.933	-262.467	-170.757	21.952
1800	34.491	62.901	35.467	49.382	-261.109	-165.390	20.081
1900	34.491	64.766	36.960	52.831	-259.772	-160.109	18.417
1992.2	34.491	66.400	38.285	56.011	-258.556	-155.314	17.038
1992.2	19.389	98.282	38.285	119.527	-195.040	-155.314	17.038
2000	19.393	98.358	38.519	119.678	-195.056	-155.158	16.955

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1117 K, melting point of $LiBO_2$; ΔH° = 8.080 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.
1992.2 K, boiling point of $LiBO_2$; ΔH° = 63.516 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1117 K: $C_p^\circ = 13.446 + 12.678\times10^{-3}T - 2.488\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 13.446\times10^{-3}T + 6.339\times10^{-6}T^2 + 2.488\times10^{2}T^{-1} - 5.407$
1117-1992.2 K: $C_p^\circ = 34.491$
$H^\circ - H^\circ_{298} = 34.491\times10^{-3}T - 12.702$
1992.2-2000 K: $C_p^\circ = 19.359$
$H^\circ - H^\circ_{298} = 19.359\times10^{-3}T + 80.960$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -243.729 - 0.206\times10^{-3}T - 0.314\times10^{-6}T^2 + 65.100T^{-1}$
$\Delta Gf^\circ = -243.729 + 0.206\times10^{-3}T\ln T + 0.314\times10^{-6}T^2 + 32.550T^{-1} + 43.804\times10^{-3}T$
453.7-1117 K: $\Delta Hf^\circ = -243.289 - 5.304\times10^{-3}T + 5.150\times10^{-6}T^2 + 79.400T^{-1}$
$\Delta Gf^\circ = -243.289 + 5.304\times10^{-3}T\ln T - 5.150\times10^{-6}T^2 + 39.700T^{-1} + 14.093\times10^{-3}T$
1117-1638 K: $\Delta Hf^\circ = -250.585 + 15.741\times10^{-3}T - 1.189\times10^{-6}T^2 - 169.400T^{-1}$
$\Delta Gf^\circ = -250.585 - 15.741\times10^{-3}T\ln T + 1.189\times10^{-6}T^2 - 84.700T^{-1} + 161.345\times10^{-3}T$
1638-1992.2 K: $\Delta Hf^\circ = -288.051 + 17.327\times10^{-3}T - 1.173\times10^{-6}T^2 - 717.300T^{-1}$
$\Delta Gf^\circ = -288.051 - 17.327\times10^{-3}T\ln T + 1.173\times10^{-6}T^2 - 358.650T^{-1} + 196.085\times10^{-3}T$
1992.2-2000 K: $\Delta Hf^\circ = -194.389 + 2.195\times10^{-3}T - 1.173\times10^{-6}T^2 - 717.300T^{-1}$
$\Delta Gf^\circ = -194.389 - 2.195\times10^{-3}T\ln T + 1.173\times10^{-6}T^2 - 358.650T^{-1} + 34.113\times10^{-3}T$

Source: Data from Chase (81).

$LiBO_2(g)$
Lithium Borate (ideal gas)
[Formation: $Li(c,l,g) + B(\beta) + O_2(g) = LiBO_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	13.682	65.634	65.634	0	-154.600	-157.064	115.130
300	13.711	65.719	65.636	.025	-154.604	-157.079	114.431
400	15.013	69.852	66.189	1.465	-154.812	-157.875	86.258
453.7	15.519	71.780	66.738	2.287	-154.955	-158.277	76.242
453.7	15.519	71.780	66.738	2.287	-155.672	-158.277	76.242
500	15.955	73.309	67.277	3.016	-155.817	-158.534	69.294
600	16.668	76.283	68.535	4.649	-156.127	-159.049	57.933
700	17.221	78.896	69.833	6.344	-156.428	-159.512	49.801
800	17.657	81.225	71.114	8.089	-156.719	-159.933	43.691
900	18.002	83.326	72.356	9.873	-157.009	-160.316	38.930
1000	18.279	85.237	73.550	11.687	-157.300	-160.668	35.114
1100	18.503	86.990	74.693	13.527	-157.591	-160.996	31.986
1200	18.685	88.608	75.786	15.386	-157.887	-161.291	29.375
1300	18.835	90.110	76.831	17.263	-158.186	-161.560	27.160
1400	18.959	91.510	77.829	19.153	-158.493	-161.807	25.259
1500	19.063	92.822	78.786	21.054	-158.808	-162.030	23.607
1600	19.151	94.055	79.702	22.965	-159.133	-162.245	22.161
1638	19.179	94.505	80.040	23.693	-159.259	-162.318	21.657
1638	19.179	94.505	80.040	23.693	-194.419	-162.318	21.657
1700	19.226	95.219	80.581	24.884	-194.516	-161.099	20.710
1800	19.290	96.320	81.426	26.810	-194.681	-159.117	19.319
1900	19.345	97.364	82.237	28.741	-194.862	-157.136	18.074
2000	19.393	98.358	83.019	30.678	-195.056	-155.158	16.955

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.612 + 1.700\times10^{-3}T - 3.056\times10^{5}T^{-2}$

$H° - H°_{298} = 16.612\times10^{-3}T + 0.850\times10^{-6}T^{2} + 3.056\times10^{2}T^{-1} - 6.053$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -155.376 + 2.960\times10^{-3}T - 5.803\times10^{-6}T^{2} + 121.900T^{-1}$

$\Delta Gf° = -155.376 - 2.960\times10^{-3}T\ln T + 5.803\times10^{-6}T^{2} + 60.950T^{-1} + 8.785\times10^{-3}T$

453.7-1638 K: $\Delta Hf° = -154.936 - 2.138\times10^{-3}T - 0.339\times10^{-6}T^{2} + 136.200T^{-1}$

$\Delta Gf° = -154.936 + 2.138\times10^{-3}T\ln T + 0.339\times10^{-6}T^{2} + 68.100T^{-1} - 20.926\times10^{-3}T$

1638-2000 K: $\Delta Hf° = -192.402 - 0.552\times10^{-3}T - 0.323\times10^{-6}T^{2} - 411.700T^{-1}$

$\Delta Gf° = -192.402 + 0.552\times10^{-3}T\ln T + 0.323\times10^{-6}T^{2} - 205.850T^{-1} + 13.813\times10^{-3}T$

Source: Data from Chase (81).

$Li_2B_4O_7(c,l)$
Lithium Diborate
[Formation: $2Li(c,l,g) + 4B(\beta) + 3.5O_2(g) = Li_2B_4O_7(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	43.750	37.200	37.200	0	-810.300	-764.425	560.331
300	43.761	37.471	37.201	.081	-810.307	-764.136	556.666
400	47.239	50.492	38.952	4.616	-810.766	-748.690	409.060
453.7	50.100	56.622	40.683	7.231	-811.086	-740.331	356.617
453.7	50.100	56.622	40.683	7.231	-812.520	-740.331	356.617
500	52.567	61.610	42.394	9.608	-812.797	-732.945	320.366
600	57.625	71.653	46.446	15.124	-813.249	-716.938	261.141
700	61.950	80.869	50.715	21.108	-813.461	-700.862	218.816
800	65.586	89.384	55.023	27.489	-813.440	-684.775	187.069
900	68.766	97.294	59.285	34.208	-813.228	-668.701	162.381
1000	71.803	104.695	63.461	41.234	-812.829	-652.661	142.637
1100	75.052	111.691	67.529	48.578	-812.214	-636.693	126.498
1190	77.883	117.703	71.089	55.470	-811.456	-622.344	114.295
1190	111.778	142.039	71.089	84.430	-782.496	-622.344	114.295
1200	111.845	142.974	71.682	85.550	-782.062	-620.998	113.098
1300	112.515	151.953	77.516	96.768	-777.747	-607.738	102.169
1400	113.156	160.316	83.136	108.052	-773.449	-594.824	92.855
1500	113.728	168.142	88.545	119.396	-769.169	-582.200	84.825
1600	114.315	175.500	93.751	130.798	-764.910	-569.920	77.847
1638	114.544	178.186	95.679	135.146	-763.294	-565.310	75.425
1638	114.544	178.186	95.679	135.146	-833.614	-565.310	75.425
1700	114.918	182.449	98.767	142.260	-830.759	-555.199	71.375
1800	115.537	189.035	103.601	153.782	-826.163	-539.074	65.452
1900	116.172	195.298	108.262	165.368	-821.582	-523.245	60.186
2000	116.822	201.274	112.766	177.017	-817.012	-507.713	55.480

*Entropy at 298 K estimated and heat capacities extrapolated above 1373 K.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1190 K, melting point of $Li_2B_4O_7$; ΔH° = 28.960 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1190 K: $Cp° = 34.372 + 38.058\times10^{-3}T - 1.750\times10^{5}T^{-2}$
$H°-H°_{298} = 34.372\times10^{-3}T + 19.029\times10^{-6}T^{2} + 1.750\times10^{2}T^{-1} - 12.527$
1190-2000 K: $Cp° = 107.268 + 4.882\times10^{-3}T - 18.416\times10^{5}T^{-2}$
$H°-H°_{298} = 107.268\times10^{-3}T + 2.441\times10^{-6}T^{2} + 18.416\times10^{2}T^{-1} - 48.223$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -804.318 - 13.223\times10^{-3}T + 3.585\times10^{-6}T^{2} - 703.200T^{-1}$
$\Delta Gf° = -804.318 + 13.223\times10^{-3}T\ln T - 3.585\times10^{-6}T^{2} - 351.600T^{-1} + 63.485\times10^{-3}T$
453.7-1190 K: $\Delta Hf° = -803.438 - 23.419\times10^{-3}T + 14.513\times10^{-6}T^{2} - 674.600T^{-1}$
$\Delta Gf° = -803.438 + 23.419\times10^{-3}T\ln T - 14.513\times10^{-6}T^{2} - 337.300T^{-1} + 4.062\times10^{-3}T$
1190-1638 K: $\Delta Hf° = -839.135 + 49.477\times10^{-3}T - 2.075\times10^{-6}T^{2} + 992.000T^{-1}$
$\Delta Gf° = -839.135 - 49.477\times10^{-3}T\ln T + 2.075\times10^{-6}T^{2} + 496.000T^{-1} + 529.959\times10^{-3}T$
1638-2000 K: $\Delta Hf° = -914.067 + 52.649\times10^{-3}T - 2.044\times10^{-6}T^{2} - 103.800T^{-1}$
$\Delta Gf° = -914.067 - 52.649\times10^{-3}T\ln T + 2.044\times10^{-6}T^{2} - 51.900T^{-1} + 599.439\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127) who estimated entropy at 298 K and extrapolated heat capacities above 1373 K.

$Li_2B_6O_{10}$(c)
Lithium Triborate
[Formation: $2Li(c,l) + 6B(\beta) + 5O_2(g) = Li_2B_6O_{10}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	70.080	45.000	45.000	0	-1118.600	-1052.294	771.342
300	70.180	45.434	45.001	.130	-1118.587	-1051.876	766.281
400	75.590	66.378	47.820	7.423	-1117.988	-1029.748	562.621
453.7	78.194	76.072	50.597	11.558	-1117.791	-1017.905	490.324
453.7	78.194	76.072	50.597	11.558	-1119.225	-1017.905	490.324
500	80.440	83.779	53.319	15.230	-1119.114	-1007.566	440.401
600	84.610	98.824	59.676	23.489	-1118.906	-985.290	358.887
700	88.050	112.132	66.238	32.126	-1118.667	-963.032	300.668
800	90.940	124.083	72.734	41.079	-1118.364	-940.818	257.016
900	93.390	134.939	79.051	50.299	-1118.010	-918.642	223.074
1000	95.500	144.890	85.145	59.745	-1117.607	-896.509	195.929
1100	97.145	154.069	90.999	69.377	-1117.170	-874.454	173.736

*Entropy at 298 K estimated and heat capacities extrapolated above 823 K.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1107 K, incongruent melting point of $Li_2B_6O_{10}$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 72.123 + 23.960\times10^{-3}T - 8.166\times10^{5}T^{-2}$
$H° - H^\circ_{298} = 72.123\times10^{-3}T + 11.980\times10^{-6}T^{2} + 8.166\times10^{2}T^{-1} - 25.307$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -1117.445 + 4.237\times10^{-3}T - 5.603\times10^{-6}T^{2} - 572.400T^{-1}$
$\Delta Gf° = -1117.445 - 4.237\times10^{-3}T\ln T + 5.603\times10^{-6}T^{2} - 286.200T^{-1} + 244.211\times10^{-3}T$
453.7-1100 K: $\Delta Hf° = -1116.566 - 5.959\times10^{-3}T + 5.325\times10^{-6}T^{2} - 543.800T^{-1}$
$\Delta Gf° = -1116.566 + 5.959\times10^{-3}T\ln T - 5.325\times10^{-6}T^{2} - 271.900T^{-1} + 184.787\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127) who estimated entropy at 298 K and extrapolated heat capacities above 823 K.

$Li_2B_8O_{13}(c)$
Lithium Tetraborate
[Formation: $2Li(c,l) + 8B(\beta) + 6.5O_2(g) = Li_2B_8O_{13}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	77.800	63.400	63.400	0	-1420.000	-1336.422	979.611
300	78.100	63.882	63.402	.144	-1420.002	-1335.895	973.187
400	93.300	88.577	66.665	8.765	-1419.775	-1307.896	714.592
453.7	98.203	100.689	69.979	13.933	-1419.548	-1292.874	622.777
453.7	98.203	100.689	69.979	13.933	-1420.982	-1292.874	622.777
500	102.430	110.437	73.281	18.578	-1420.805	-1279.805	559.395
600	108.320	129.656	81.109	29.128	-1420.388	-1251.665	455.913
700	112.700	146.692	89.283	40.186	-1419.932	-1223.568	382.010
800	116.320	161.986	97.432	51.643	-1419.414	-1195.550	326.605
900	119.200	175.858	105.388	63.423	-1418.859	-1167.597	283.528

*Entropy at 298 K estimated.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
908 K, incongruent melting point of $Li_2B_8O_{13}$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp^\circ = 99.475 + 25.900\text{x}10^{-3}T - 26.132\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 99.475\text{x}10^{-3}T + 12.950\text{x}10^{-6}T^2 + 26.132\text{x}10^{2}T^{-1} - 39.574$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -1425.159 + 11.298\text{x}10^{-3}T - 6.772\text{x}10^{-6}T^2 + 713.400T^{-1}$
$\Delta Gf^\circ = -1425.159 - 11.298\text{x}10^{-3}T\ln T + 6.772\text{x}10^{-6}T^2 + 356.700T^{-1} + 355.965\text{x}10^{-3}T$
453.7-900 K: $\Delta Hf^\circ = -1424.280 + 1.102\text{x}10^{-3}T + 4.157\text{x}10^{-6}T^2 + 742.000T^{-1}$
$\Delta Gf^\circ = -1424.280 - 1.102\text{x}10^{-3}T\ln T - 4.157\text{x}10^{-6}T^2 + 371.000T^{-1} + 296.542\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Shul'ts (457). Other data from JANAF (127) who estimated entropy at 298 K.

$LiBeF_3(c)$
Lithium Trifluoroberyllate
[Formation: $Li(c,l) + Be(c) + 1.5F_2(g) = LiBeF_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	21.945	21.330	21.330	0	-394.300	-376.244	275.791
300	22.000	21.466	21.330	.041	-394.298	-376.134	274.010
400	25.000	28.206	22.229	2.391	-394.159	-370.095	202.208
453.7	26.611	31.454	23.129	3.777	-394.044	-366.876	176.724
453.7	26.611	31.454	23.129	3.777	-394.761	-366.876	176.724
500	28.000	34.107	24.025	5.041	-394.634	-364.035	159.117
600	31.000	39.477	26.159	7.991	-394.186	-357.949	130.381

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 13.000 + 30.000x10^{-3}T$

$H°- H°_{298} = 13.000x10^{-3}T + 15.000x10^{-6}T^2 - 5.209$

Formation equations (kcal/mol):

298.15-453.7 K: $ΔHf° = -392.550 - 6.202x10^{-3}T + 8.319x10^{-6}T^2 - 190.850T^{-1}$

$ΔGf° = -392.550 + 6.202x10^{-3}TlnT - 8.319x10^{-6}T^2 - 95.425T^{-1} + 22.907x10^{-3}T$

453.7-600 K: $ΔHf° = -392.111 - 11.300x10^{-3}T + 13.783x10^{-6}T^2 - 176.550T^{-1}$

$ΔGf° = -392.111 + 11.300x10^{-3}TlnT - 13.783x10^{-6}T^2 - 88.275T^{-1} - 6.804x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data are those estimated by Chase (81).

Li_2BeF_4(c,l)
Dilithium Tetrafluoroberyllate
[Formation: $2Li(c,l) + Be(c) + 2F_2(g) = Li_2BeF_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	32.330	31.210	31.210	0	-543.900	-519.495	380.795
300	32.390	31.410	31.210	.060	-543.897	-519.346	378.338
400	35.960	41.217	32.524	3.477	-543.696	-511.188	279.296
453.7	37.872	45.864	33.831	5.459	-543.566	-506.839	244.144
453.7	37.872	45.864	33.831	5.459	-545.000	-506.839	244.144
500	39.520	49.624	35.122	7.251	-544.867	-502.946	219.835
600	43.080	57.144	38.176	11.381	-544.368	-494.599	180.155
700	46.650	64.053	41.384	15.868	-543.552	-486.370	151.850
732.2	47.800	66.177	42.427	17.390	-543.218	-483.746	144.388
732.2	55.470	80.538	42.427	27.905	-532.703	-483.746	144.388
800	55.470	85.450	45.869	31.665	-531.461	-479.269	130.929
900*	55.470	91.983	50.636	37.212	-529.655	-472.848	114.822
1000	55.470	97.827	55.068	42.759	-527.886	-466.635	101.982
1100	55.470	103.114	59.199	48.306	-526.149	-460.593	91.510
1200	55.470	107.941	63.064	53.853	-524.443	-454.717	82.814
1300	55.470	112.381	66.689	59.400	-522.764	-448.967	75.477
1400	55.470	116.492	70.101	64.947	-521.115	-443.353	69.210
1500	55.470	120.319	73.323	70.494	-519.489	-437.867	63.796

*Heat capacities extrapolated above 873 K.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
732.2 K, melting point of Li_2BeF_4; ΔH° = 10.515 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-732.2 K: $Cp^\circ = 21.646 + 35.726\times10^{-3}T + 0.029\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 21.646\times10^{-3}T + 17.863\times10^{-6}T^2 - 0.029\times10^{2}T^{-1} - 8.032$
732.2-1500 K: $Cp^\circ = 55.470$
$H^\circ - H^\circ_{298} = 55.470\times10^{-3}T - 12.710$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -542.815 - 3.509\times10^{-3}T + 5.637\times10^{-6}T^2 - 161.000T^{-1}$
$\Delta Gf^\circ = -542.815 + 3.509\times10^{-3}T\ln T - 5.637\times10^{-6}T^2 - 80.500T^{-1} + 60.808\times10^{-3}T$
453.7-732.2 K: $\Delta Hf^\circ = -541.936 - 13.705\times10^{-3}T + 16.565\times10^{-6}T^2 - 132.400T^{-1}$
$\Delta Gf^\circ = -541.936 + 13.705\times10^{-3}T\ln T - 16.565\times10^{-6}T^2 - 66.200T^{-1} + 1.385\times10^{-3}T$
732.2-1500 K: $\Delta Hf^\circ = -546.614 + 20.119\times10^{-3}T - 1.298\times10^{-6}T^2 - 129.500T^{-1}$
$\Delta Gf^\circ = -546.614 - 20.119\times10^{-3}T\ln T + 1.298\times10^{-6}T^2 - 64.750T^{-1} + 217.797\times10^{-3}T$

Sources: Enthalpy of formation from Wagman (516). Other data are from Chase (81) who extrapolated heat capacities above 873 K.

Li_2C_2(c)
Dilithium Dicarbide
[Formation: $2Li(c,l,g) + 2C(c) = Li_2C_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	17.100	14.000	14.000	0	-14.200	-13.409	9.829
300	17.200	14.106	14.000	.032	-14.198	-13.405	9.765
400	20.890	19.630	14.727	1.961	-13.999	-13.165	7.193
453.7	21.873	22.341	15.470	3.118	-13.899	-13.066	6.294
453.7	21.873	22.341	15.470	3.118	-15.333	-13.066	6.294
500	22.720	24.508	16.208	4.150	-15.280	-12.832	5.609
600	23.830	28.756	17.953	6.482	-15.128	-12.354	4.500
700	24.600	32.491	19.768	8.906	-14.952	-11.908	3.718
800	25.180	35.815	21.570	11.396	-14.764	-11.485	3.137
900	25.660	38.810	23.323	13.938	-14.578	-11.090	2.693
1000	26.070	41.535	25.010	16.525	-14.385	-10.712	2.341
1100	26.430	44.037	26.627	19.151	-14.183	-10.332	2.053
1200	26.770	46.352	28.176	21.811	-13.975	-10.015	1.824
1300	27.090	48.507	29.658	24.504	-13.754	-9.694	1.630
1400	27.390	50.525	31.076	27.228	-13.518	-9.389	1.466
1500	27.680	52.425	32.437	29.982	-13.266	-9.103	1.326
1600	27.960	54.221	33.743	32.764	-12.994	-8.832	1.206
1638	28.066	54.879	34.226	33.829	-12.886	-8.737	1.166
1638	28.066	54.879	34.226	33.829	-83.206	-8.737	1.166
1700	28.240	55.924	34.998	35.574	-82.804	-5.923	.761
1800	28.510	57.546	36.207	38.411	-82.135	-1.419	.172
1900	28.780	59.094	37.370	41.276	-81.450	3.047	-.350
2000	29.040	60.577	38.493	44.167	-80.751	7.479	-.817

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.334 + 2.442 \times 10^{-3}T - 7.078 \times 10^{5}T^{-2}$
$H° - H°_{298} = 24.334 \times 10^{-3}T + 1.221 \times 10^{-6}T^{2} + 7.078 \times 10^{2}T^{-1} - 9.738$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -19.121 + 13.900 \times 10^{-3}T - 11.227 \times 10^{-6}T^{2} + 529.200T^{-1}$
$\Delta Gf° = -19.121 - 13.900 \times 10^{-3}T\ln T + 11.227 \times 10^{-6}T^{2} + 264.600T^{-1} + 92.031 \times 10^{-3}T$
453.7-1638 K: $\Delta Hf° = -18.242 + 3.704 \times 10^{-3}T - 0.299 \times 10^{-6}T^{2} + 557.800T^{-1}$
$\Delta Gf° = -18.242 - 3.704 \times 10^{-3}T\ln T + 0.299 \times 10^{-6}T^{2} + 278.900T^{-1} + 32.607 \times 10^{-3}T$
1638-2000 K: $\Delta Hf° = -93.174 + 6.876 \times 10^{-3}T - 0.267 \times 10^{-6}T^{2} - 538.000T^{-1}$
$\Delta Gf° = -93.174 - 6.876 \times 10^{-3}T\ln T + 0.267 \times 10^{-6}T^{2} - 269.000T^{-1} + 102.087 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127).

$Li_2CO_3(c,l)$
Lithium Carbonate
[Formation: $2Li(c,l,g) + C(c) + 1.5O_2(g) = Li_2CO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	23.000	21.551	21.551	0	-290.640	-270.593	198.348
300	23.080	21.694	21.551	.043	-290.643	-270.469	197.034
400	26.810	28.860	22.503	2.543	-290.694	-263.731	144.094
453.7	28.963	32.354	23.463	4.034	-290.681	-260.116	125.298
453.7	28.963	32.354	23.463	4.034	-292.115	-260.116	125.298
500	30.820	35.259	24.423	5.418	-292.068	-256.848	112.267
600	35.700	41.295	26.735	8.736	-291.686	-249.832	91.000
623	36.600	42.656	27.301	9.566	-291.539	-248.232	87.079
623	38.700	42.871	27.301	9.700	-291.405	-248.232	87.079
683	38.700	46.430	28.831	12.020	-290.881	-244.104	78.109
683	32.920	47.213	28.831	12.555	-290.346	-244.104	78.109
700	33.670	48.033	29.280	13.127	-290.285	-242.948	75.851
800	38.000	52.811	31.922	16.711	-289.742	-236.218	64.531
900	42.310	57.535	34.506	20.726	-288.816	-229.580	55.749
993.15	46.367	61.902	36.875	24.856	-287.599	-223.511	49.185
993.15	44.320	72.676	36.875	35.556	-276.899	-223.511	49.185
1000	44.320	72.980	37.121	35.859	-276.811	-223.143	48.767
1100	44.320	77.204	40.576	40.291	-275.538	-217.826	43.277
1200	44.320	81.061	43.792	44.723	-274.292	-212.648	38.728
1300	44.320	84.608	46.796	49.155	-273.066	-207.560	34.894
1400	44.320	87.893	49.617	53.587	-271.859	-202.568	31.622
1500	44.320	90.951	52.272	58.019	-270.666	-197.661	28.799
1600	44.320	93.811	54.779	62.451	-269.485	-192.830	26.339
1638	44.320	94.851	55.697	64.135	-269.039	-191.016	25.486
1638	44.320	94.851	55.697	64.135	-339.359	-191.016	25.486
1700	44.320	96.498	57.155	66.883	-338.414	-185.416	23.837
1800	44.320	99.031	59.412	71.315	-336.895	-176.457	21.425
1900	44.320	101.427	61.560	75.747	-335.392	-167.587	19.277
2000	44.320	103.701	63.611	80.179	-333.903	-158.792	17.352

Phase changes:
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
623 K, α - β transition point of Li_2CO_3; ΔH° = 0.134 kcal/mol.
683 K, β - γ transition point of Li_2CO_3; ΔH° = 0.535 kcal/mol.
993.15 K, melting point of Li_2CO_3; ΔH° = 10.700 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-623 K: $Cp° = 7.126 + 46.320\times10^{-3}T + 1.835\times10^{5}T^{-2}$
$H°-H°_{298} = 7.126\times10^{-3}T + 23.160\times10^{-6}T^2 - 1.835\times10^{2}T^{-1} - 3.568$
623-683 K: $Cp° = 38.666$
$H°-H°_{298} = 38.666\times10^{-3}T - 14.389$
683-993.15 K: $Cp° = 8.093 + 39.348\times10^{-3}T - 9.554\times10^{5}T^{-2}$
$H°-H°_{298} = 8.093\times10^{-3}T + 19.674\times10^{-6}T^2 + 9.554\times10^{2}T^{-1} - 3.549$
993.15-2000 K: $Cp° = 44.320$
$H°-H°_{298} = 44.320\times10^{-3}T - 8.460$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -287.558 - 10.635\times10^{-3}T + 10.723\times10^{-6}T^2 - 257.600T^{-1}$
$\Delta Gf° = -287.558 + 10.635\times10^{-3}T\ln T - 10.723\times10^{-6}T^2 - 128.800T^{-1} + 0.953\times10^{-3}T$
453.7-623 K: $\Delta Hf° = -286.679 - 20.831\times10^{-3}T + 21.651\times10^{-6}T^2 - 229.000T^{-1}$
$\Delta Gf° = -286.679 + 20.831\times10^{-3}T\ln T - 21.651\times10^{-6}T^2 - 114.500T^{-1} - 58.470\times10^{-3}T$
623-683 K: $\Delta Hf° = -297.500 + 10.709\times10^{-3}T - 1.509\times10^{-6}T^2 - 45.500T^{-1}$
$\Delta Gf° = -297.500 - 10.709\times10^{-3}T\ln T + 1.509\times10^{-6}T^2 - 22.750T^{-1} + 147.179\times10^{-3}T$
683-993.15 K: $\Delta Hf° = -286.660 - 19.864\times10^{-3}T + 18.165\times10^{-6}T^2 + 909.900T^{-1}$
$\Delta Gf° = -286.660 + 19.864\times10^{-3}T\ln T - 18.165\times10^{-6}T^2 + 454.950T^{-1} - 55.813\times10^{-3}T$
993.15-1638 K: $\Delta Hf° = -291.572 + 16.363\times10^{-3}T - 1.509\times10^{-6}T^2 - 45.500T^{-1}$
$\Delta Gf° = -291.572 - 16.363\times10^{-3}T\ln T + 1.509\times10^{-6}T^2 - 22.750T^{-1} + 180.076\times10^{-3}T$
1638-2000 K: $\Delta Hf° = -366.504 + 19.535\times10^{-3}T - 1.477\times10^{-6}T^2 - 1141.300T^{-1}$
$\Delta Gf° = -366.504 - 19.535\times10^{-3}T\ln T + 1.477\times10^{-6}T^2 - 570.650T^{-1} + 249.556\times10^{-3}T$

Source: Data from Chang (74).

$LiClO_4(c,l)$
Lithium Perchlorate
[Formation: $Li(c,l) + 0.5Cl_2g) + 2O_2g) = LiClO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.952	28.537	28.537	0	-91.060	-60.329	44.222
300	25.072	28.704	28.537	.050	-91.054	-60.138	43.810
400	29.995	36.580	29.568	2.805	-90.756	-49.861	27.242
453.7	32.370	40.507	30.615	4.488	-90.445	-44.383	21.379
453.7	32.370	40.507	30.615	4.488	-91.162	-44.383	21.379
500	34.417	43.752	31.684	6.034	-90.833	-39.623	17.319
520.7	35.277	45.176	32.197	6.758	-90.656	-37.509	15.743
520.7	38.313	54.375	32.197	11.548	-85.866	-37.509	15.743
600	39.089	59.859	35.497	14.617	-84.908	-30.213	11.005
700*	40.067	65.958	39.424	18.574	-83.646	-21.198	6.618
800	41.046	71.372	43.085	22.630	-82.321	-12.368	3.379
900	42.025	76.263	46.503	26.784	-80.931	-3.706	.900
1000	43.003	80.741	49.706	31.035	-79.470	4.797	-1.048

*Data extrapolated above 600 K.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
520.7 K, melting point of $LiClO_4$; ΔH° = 4.790 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-520.7 K: $Cp° = 14.571 + 41.268\text{x}10^{-3}T - 1.710\text{x}10^{5}T^{-2}$
$H°- H°_{298} = 14.571\text{x}10^{-3}T + 20.634\text{x}10^{-6}T^{2} + 1.710\text{x}10^{2}T^{-1} - 6.752$
520.7-1000 K: $Cp° = 33.217 + 9.786\text{x}10^{-3}T$
$H°- H°_{298} = 33.217\text{x}10^{-3}T + 4.893\text{x}10^{-6}T^{2} - 7.075$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -90.961 - 6.002\text{x}10^{-3}T + 14.126\text{x}10^{-6}T^{2} + 129.450T^{-1}$
$\Delta Gf° = -90.961 + 6.002\text{x}10^{-3}T\ln T - 14.126\text{x}10^{-6}T^{2} + 64.725T^{-1} + 72.028\text{x}10^{-3}T$
453.7-520.7 K: $\Delta Hf° = -90.521 - 11.100\text{x}10^{-3}T + 19.590\text{x}10^{-6}T^{2} + 143.750T^{-1}$
$\Delta Gf° = -90.521 + 11.100\text{x}10^{-3}T\ln T - 19.590\text{x}10^{-6}T^{2} + 71.875T^{-1} + 42.316\text{x}10^{-3}T$
520.7-1000 K: $\Delta Hf° = -90.844 + 7.546\text{x}10^{-3}T + 3.849\text{x}10^{-6}T^{2} - 27.250T^{-1}$
$\Delta Gf° = -90.844 - 7.546\text{x}10^{-3}T\ln T - 3.849\text{x}10^{-6}T^{2} - 13.625T^{-1} + 151.689\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy from Zalukaev (540). High-temperature data based on Schmidt (447). Data extrapolated above 600 K.

$LiFeO_2(c)$
Lithium Ferrite
[Formation: $Li(c,l,g) + Fe(c,l) + O_2(g) = LiFeO_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.810	18.000	18.000	0	-179.300	-166.039	121.708
300	19.860	18.123	18.000	.037	-179.298	-165.956	120.897
400	21.846	24.133	18.806	2.131	-179.161	-161.527	88.253
453.7	22.507	26.934	19.604	3.326	-179.081	-159.167	76.671
453.7	22.507	26.934	19.604	3.326	-179.798	-159.167	76.671
500	23.076	29.149	20.387	4.381	-179.742	-157.062	68.651
600	23.922	33.435	22.213	6.733	-179.595	-152.539	55.561
700	24.541	37.172	24.089	9.158	-179.443	-148.042	46.220
800	25.019	40.481	25.935	11.637	-179.319	-143.566	39.220
900	25.412	43.451	27.719	14.159	-179.264	-139.101	33.778
1000	25.765	46.147	29.429	16.718	-179.358	-134.636	29.424
1043	25.916	47.235	30.141	17.829	-179.536	-132.710	27.808
1100	26.116	48.619	31.063	19.312	-179.623	-130.146	25.857
1185	26.442	50.574	32.393	21.545	-179.579	-126.325	23.298
1185	26.442	50.574	32.393	21.545	-179.794	-126.325	23.298
1200	26.500	50.907	32.622	21.942	-179.750	-125.649	22.884
1300	26.948	53.046	34.112	24.614	-179.440	-121.153	20.367
1400	27.490	55.062	35.537	27.335	-179.109	-116.682	18.215
1500	28.154	56.980	36.903	30.116	-178.742	-112.235	16.352
1600	28.967	58.823	38.216	32.971	-178.326	-107.814	14.727
1638	29.342	59.507	38.702	34.079	-178.151	-106.143	14.162
1638	29.342	59.507	38.702	34.079	-213.311	-106.143	14.162
1667	29.628	60.023	39.068	34.932	-213.119	-104.246	13.667
1667	29.628	60.023	39.068	34.932	-213.319	-104.246	13.667
1700	29.954	60.607	39.481	35.915	-213.119	-102.087	13.124
1800	31.141	62.352	40.703	38.968	-212.451	-95.573	11.604
1811	31.296	62.542	40.835	39.311	-212.375	-94.862	11.448
1811	31.296	62.542	40.835	39.311	-215.675	-94.862	11.448
1900	32.550	64.072	41.887	42.151	-215.054	-88.940	10.230
2000	34.205	65.783	43.040	45.486	-214.216	-82.324	8.996

Phase changes:
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 21.461 + 4.858\times10^{-3}T - 2.755\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 21.461\times10^{-3}T + 2.429\times10^{-6}T^2 + 2.755\times10^{2}T^{-1} - 7.539$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -184.066 + 12.753\times10^{-3}T - 9.603\times10^{-6}T^2 + 541.800T^{-1}$
$\Delta Gf^\circ = -184.066 - 12.753\times10^{-3}T\ln T + 9.603\times10^{-6}T^2 + 270.900T^{-1} + 127.215\times10^{-3}T$
453.7-1043 K: $\Delta Hf^\circ = -183.626 + 7.655\times10^{-3}T - 4.139\times10^{-6}T^2 + 556.100T^{-1}$
$\Delta Gf^\circ = -183.626 - 7.655\times10^{-3}T\ln T + 4.139\times10^{-6}T^2 + 278.050T^{-1} + 97.503\times10^{-3}T$
1043-1185 K: $\Delta Hf^\circ = -160.065 - 36.326\times10^{-3}T + 16.572\times10^{-6}T^2 + 327.600T^{-1}$
$\Delta Gf^\circ = -160.065 + 36.326\times10^{-3}T\ln T - 16.572\times10^{-6}T^2 + 163.800T-1- 209.041\times10^{-3}T$
1185-1638 K: $\Delta Hf^\circ = -183.679 + 1.929\times10^{-3}T + 0.881\times10^{-6}T^2 + 446.600T^{-1}$
$\Delta Gf^\circ = -183.679 - 1.929\times10^{-3}T\ln T - 0.881\times10^{-6}T^2 + 223.300T^{-1} + 62.999\times10^{-3}T$
1638-1667 K: $\Delta Hf^\circ = -221.146 + 3.515\times10^{-3}T + 0.897\times10^{-6}T^2 - 101.300T^{-1}$
$\Delta Gf^\circ = -221.146 - 3.515\times10^{-3}T\ln T - 0.897\times10^{-6}T^2 - 50.650T^{-1} + 97.739\times10^{-3}T$
1667-1811 K: $\Delta Hf^\circ = -304.040 + 52.012\times10^{-3}T - 8.734\times10^{-6}T^2 + 47597.900T^{-1}$
$\Delta Gf^\circ = -304.040 - 52.012\times10^{-3}T\ln T + 8.734\times10^{-6}T^2 + 23798.950T^{-1} + 482.617\times10^{-3}T$
1811-2000 K: $\Delta Hf^\circ = -218.191 - 1.980\times10^{-3}T + 1.948\times10^{-6}T^2 - 220.300T^{-1}$
$\Delta Gf^\circ = -218.191 + 1.980\times10^{-3}T\ln T - 1.948\times10^{-6}T^2 - 110.150T^{-1} + 56.820\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from King (260). High-temperature data based on Christensen (93) and Landiya (295).

LiH(c,l)
Lithium Hydride
[Formation: Li(c,l) + $0.5H_2$(g) = LiH(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	6.700	4.790	4.790	0	-21.640	-16.343	11.979
300	6.800	4.830	4.790	.012	-21.646	-16.310	11.882
400	8.500	7.160	5.088	.829	-21.796	-14.501	7.923
453.7	9.252	8.309	5.399	1.321	-21.859	-13.519	6.512
453.7	9.252	8.309	5.399	1.321	-22.576	-13.519	6.512
500	9.900	9.240	5.712	1.764	-22.629	-12.590	5.503
600	11.000	11.130	6.457	2.804	-22.652	-10.576	3.852
700	12.000	12.890	7.246	3.951	-22.556	-8.566	2.674
800	13.100	14.560	8.056	5.203	-22.349	-6.580	1.797
900	14.200	16.160	8.869	6.562	-22.037	-4.627	1.124
962	15.200	17.160	9.369	7.495	-21.754	-3.436	.781
962	16.800	22.640	9.371	12.765	-16.484	-3.436	.781
1000	16.500	23.290	9.887	13.403	-16.244	-2.925	.639
1100	15.700	24.830	11.178	15.017	-15.681	-1.622	.322
1200	14.800	26.160	12.372	16.546	-15.208	-.365	.066
1300	13.900	27.310	13.473	17.988	-14.825	.862	-.145

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
962 K, melting point of LiH; ΔH° = 5.270 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-962 K: $Cp° = 6.874 + 8.314\times10^{-3}T - 2.358\times10^{5}T^{-2}$
$H°-H°_{298} = 6.874\times10^{-3}T + 4.157\times10^{-6}T^2 + 2.358\times10^{2}T^{-1} - 3.210$
962-1300 K: $Cp° = 31.564 - 12.300\times10^{-3}T - 27.117\times10^{5}T^{-2}$
$H°-H°_{298} = 31.564\times10^{-3}T - 6.150\times10^{-6}T^2 + 27.117\times10^{2}T^{-1} - 14.727$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -23.183 + 1.947\times10^{-3}T - 1.510\times10^{-6}T^2 + 327.050T^{-1}$
$\Delta Gf° = -23.183 - 1.947\times10^{-3}T\ln T + 1.510\times10^{-6}T^2 + 163.525T^{-1} + 31.747\times10^{-3}T$
453.7-962 K: $\Delta Hf° = -22.743 - 3.151\times10^{-3}T + 3.954\times10^{-6}T^2 + 341.350T^{-1}$
$\Delta Gf° = -22.743 + 3.151\times10^{-3}T\ln T - 3.954\times10^{-6}T^2 + 170.675T^{-1} + 2.035\times10^{-3}T$
962-1300 K: $\Delta Hf° = -34.260 + 21.539\times10^{-3}T - 6.353\times10^{-6}T^2 + 2817.250T^{-1}$
$\Delta Gf° = -34.260 - 21.539\times10^{-3}T\ln T + 6.353\times10^{-6}T^2 + 1408.625T^{-1} + 172.350\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from Shpil'rain (455).

LiH(g)
Lithium Hydride (ideal gas)
[Formation: Li(c,l,g) + 0.5H$_2$(g) = LiH(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.106	40.821	40.821	0	33.280	27.835	-20.403
300	7.109	40.865	40.822	.013	33.275	27.800	-20.252
400	7.364	42.943	41.103	.736	33.030	26.012	-14.212
453.7	7.520	43.880	41.377	1.136	32.876	25.078	-12.080
453.7	7.520	43.880	41.377	1.136	32.159	25.078	-12.080
500	7.655	44.617	41.643	1.487	32.014	24.365	-10.650
600	7.921	46.037	42.260	2.266	31.730	22.862	-8.327
700	8.145	47.276	42.890	3.070	31.483	21.403	-6.682
800	8.329	48.376	43.508	3.894	31.262	19.978	-5.458
900	8.478	49.366	44.105	4.735	31.056	18.581	-4.512
1000	8.601	50.265	44.676	5.589	30.861	17.206	-3.760
1100	8.703	51.090	45.223	6.454	30.675	15.849	-3.149
1200	8.790	51.851	45.744	7.329	30.494	14.509	-2.642
1300	8.864	52.558	46.241	8.212	30.319	13.183	-2.216
1400	8.929	53.217	46.716	9.101	30.145	11.872	-1.853
1500	8.987	53.835	47.170	9.997	29.974	10.572	-1.540
1600	9.038	54.417	47.606	10.898	29.805	9.284	-1.268
1638	9.056	54.629	47.766	11.242	29.742	8.797	-1.174
1638	9.056	54.629	47.766	11.242	-5.418	8.797	-1.174
1700	9.085	54.966	48.022	11.805	-5.409	9.339	-1.201
1800	9.128	55.487	48.423	12.715	-5.395	10.203	-1.239
1900	9.168	55.981	48.807	13.630	-5.381	11.071	-1.273
2000	9.206	56.452	49.178	14.549	-5.367	11.938	-1.305

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.427 + 1.092\mathrm{x}10^{-3}T - 0.575\mathrm{x}10^{5}T^{-2}$
$H°- H°_{298} = 7.427\mathrm{x}10^{-3}T + 0.546\mathrm{x}10^{-6}T^{2} + 0.575\mathrm{x}10^{2}T^{-1} - 2.456$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = 32.491 + 2.500\mathrm{x}10^{-3}T - 5.121\mathrm{x}10^{-6}T^{2} + 148.750T^{-1}$
$\Delta Gf° = 32.491 - 2.500\mathrm{x}10^{-3}T\ln T + 5.121\mathrm{x}10^{-6}T^{2} + 74.375T^{-1} - 3.737\mathrm{x}10^{-3}T$
453.7-1638 K: $\Delta Hf° = 32.931 - 2.598\mathrm{x}10^{-3}T + 0.343\mathrm{x}10^{-6}T^{2} + 163.050T^{-1}$
$\Delta Gf° = 32.931 + 2.598\mathrm{x}10^{-3}T\ln T - 0.343\mathrm{x}10^{-6}T^{2} + 81.525T^{-1} - 33.448\mathrm{x}10^{-3}T$
1638-2000 K: $\Delta Hf° = -4.536 - 1.012\mathrm{x}10^{-3}T + 0.359\mathrm{x}10^{-6}T^{2} - 384.850T^{-1}$
$\Delta Gf° = -4.536 + 1.012\mathrm{x}10^{-3}T\ln T - 0.359\mathrm{x}10^{-6}T^{2} - 192.425T^{-1} + 1.292\mathrm{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127).

$Li_2MoO_4(c,l)$
Lithium Molybdate
[Formation: $2Li(c,l) + Mo(c) + 2O_2(g) = Li_2MoO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	34.230	30.000	30.000	0	-363.360	-336.894	246.947
300	34.260	30.210	30.010	.060	-363.359	-336.733	245.307
400	36.230	40.340	31.365	3.590	-363.078	-327.894	179.150
453.7	37.288	44.962	32.702	5.562	-362.940	-323.181	155.676
453.7	37.288	44.962	32.702	5.562	-364.374	-323.181	155.676
500	38.200	48.630	34.010	7.310	-364.263	-318.978	139.423
600	40.170	55.770	37.053	11.230	-363.904	-309.951	112.898
700	42.130	62.110	40.196	15.340	-363.387	-301.004	93.976
800	44.100	67.870	43.295	19.660	-362.696	-292.135	79.807
900	46.070	73.180	46.336	24.160	-361.865	-283.373	68.812
974	47.530	76.870	48.501	27.630	-361.133	-276.934	62.139
974	51.410	88.880	48.501	39.330	-349.433	-276.934	62.139
1000	51.410	90.230	49.560	40.670	-349.059	-274.995	60.099
1100	51.410	95.130	53.485	45.810	-347.657	-267.656	53.178
1200	51.410	99.610	57.152	50.950	-346.287	-260.453	47.434
1300	51.410	103.720	60.574	56.090	-344.946	-253.351	42.592
1400	51.410	107.530	63.794	61.230	-343.635	-246.355	38.457
1500	51.410	111.080	66.827	66.380	-342.340	-239.449	34.887

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
974 K, melting point of Li_2MoO_4; ΔH° = 11.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-974 K: $Cp° = 28.389 + 19.640\times10^{-3}T$
$H°-H°_{298} = 28.389\times10^{-3}T + 9.820\times10^{-6}T^2 - 9.337$
974-1500 K: $Cp° = 51.410$
$H°-H°_{298} = 51.410\times10^{-3}T - 10.743$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -365.355 + 6.154\times10^{-3}T - 3.287\times10^{-6}T^2 + 134.800T^{-1}$
$\Delta Gf° = -365.355 - 6.154\times10^{-3}T\ln T + 3.287\times10^{-6}T^2 + 67.400T^{-1} + 128.783\times10^{-3}T$
453.7-974 K: $\Delta Hf° = -364.475 - 4.042\times10^{-3}T + 7.641\times10^{-6}T^2 + 163.400T^{-1}$
$\Delta Gf° = -364.475 + 4.042\times10^{-3}T\ln T - 7.641\times10^{-6}T^2 + 81.700T^{-1} + 69.360\times10^{-3}T$
974-1500 K: $\Delta Hf° = -365.882 + 18.979\times10^{-3}T - 2.179\times10^{-6}T^2 + 163.400T^{-1}$
$\Delta Gf° = -365.882 - 18.979\times10^{-3}T\ln T + 2.179\times10^{-6}T^2 + 81.700T^{-1} + 219.656\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (516). Other data based on Denielou (118).

$LiN(g)$
Lithium Nitride (ideal gas)
[Formation: $Li(c,l,g) + 0.5N_2(g) = LiN(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	7.848	49.744	49.744	0	80.000	74.065	-54.291
300	7.857	49.793	49.744	.015	79.997	74.029	-53.929
400	8.241	52.110	50.057	.821	79.834	72.063	-39.373
453.7	8.375	53.158	50.364	1.268	79.726	71.024	-34.212
453.7	8.375	53.158	50.364	1.268	79.009	71.024	-34.212
500	8.490	53.977	50.661	1.658	78.901	70.217	-30.691
600	8.655	55.541	51.348	2.516	78.690	68.501	-24.951
700	8.772	56.884	52.044	3.388	78.498	66.818	-20.861
800	8.858	58.062	52.726	4.269	78.316	65.160	-17.801
900	8.926	59.109	53.377	5.159	78.135	63.528	-15.426
1000	8.980	60.052	53.998	6.054	77.953	61.914	-13.531
1100	9.026	60.910	54.588	6.954	77.771	60.319	-11.984
1200	9.067	61.698	55.149	7.859	77.588	58.739	-10.698
1300	9.102	62.425	55.680	8.768	77.405	57.177	-9.612
1400	9.135	63.100	56.186	9.679	77.221	55.628	-8.684
1500	9.165	63.732	56.669	10.594	77.039	54.091	-7.881
1600	9.193	64.324	57.129	11.512	76.857	52.568	-7.180
1638	9.203	64.540	57.298	11.862	76.789	51.991	-6.937
1638	9.203	64.540	57.298	11.862	41.629	51.991	-6.937
1700	9.220	64.882	57.568	12.433	41.629	52.386	-6.735
1800	9.246	65.410	57.990	13.356	41.631	53.018	-6.437
1900	9.271	65.911	58.394	14.282	41.632	53.649	-6.171
2000	9.295	66.387	58.782	15.211	41.634	54.284	-5.932
2100	9.318	66.841	59.155	16.141	41.634	54.914	-5.715
2200	9.341	67.275	59.514	17.074	41.636	55.547	-5.518
2300	9.364	67.691	59.861	18.010	41.637	56.180	-5.338
2400	9.386	68.090	60.195	18.947	41.636	56.813	-5.173
2500	9.408	68.473	60.518	19.887	41.635	57.447	-5.022

*All data estimated.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp^\circ = 8.667 + 0.352\times10^{-3}T - 0.821\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 8.667\times10^{-3}T + 0.176\times10^{-6}T^2 + 0.821\times10^{2}T^{-1} - 2.875$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = 78.823 + 3.709\times10^{-3}T - 5.576\times10^{-6}T^2 + 169.050T^{-1}$
$\Delta Gf^\circ = 78.823 - 3.709\times10^{-3}T\ln T + 5.576\times10^{-6}T^2 + 84.525T^{-1} + 2.565\times10^{-3}T$
453.7-1638 K: $\Delta Hf^\circ = 79.262 - 1.389\times10^{-3}T - 0.113\times10^{-6}T^2 + 183.350T^{-1}$
$\Delta Gf^\circ = 79.262 + 1.389\times10^{-3}T\ln T + 0.113\times10^{-6}T^2 + 91.675T^{-1} - 27.146\times10^{-3}T$
1638-2000 K: $\Delta Hf^\circ = 41.796 + 0.197\times10^{-3}T - 0.097\times10^{-6}T^2 - 364.550T^{-1}$
$\Delta Gf^\circ = 41.796 - 0.197\times10^{-3}T\ln T + 0.097\times10^{-6}T^2 - 182.275T^{-1} + 7.594\times10^{-3}T$
2000-2500 K: $\Delta Hf^\circ = 43.133 - 0.867\times10^{-3}T + 0.170\times10^{-6}T^2 - 914.500T^{-1}$
$\Delta Gf^\circ = 43.133 + 0.867\times10^{-3}T\ln T - 0.170\times10^{-6}T^2 - 457.250T^{-1} - 0.560\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$Li_3N(c)$
Trilithium Nitride
[Formation: $3Li(c,l) + 0.5N_2(g) = Li_3N(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	17.985	14.959	14.959	0	-39.330	-30.747	22.538
300	18.050	15.072	14.962	.033	-39.337	-30.695	22.361
400	20.817	20.674	15.707	1.987	-39.594	-27.771	15.173
453.7	22.080	23.376	16.456	3.139	-39.728	-26.182	12.612
453.7	22.080	23.376	16.456	3.139	-41.879	-26.182	12.612
500	23.169	25.574	17.200	4.187	-42.000	-24.567	10.738
600	25.437	30.000	18.968	6.619	-42.063	-21.069	7.674
700	27.624	34.087	20.841	9.272	-41.874	-17.585	5.490
800	29.728	37.914	22.738	12.141	-41.452	-14.141	3.863
900	31.750	41.532	24.626	15.215	-40.831	-10.762	2.613
1000	33.688	44.979	26.491	18.488	-40.015	-7.463	1.631
1086	35.289	47.823	28.068	21.454	-39.162	-4.697	.945

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1086 K, melting point of Li_3N; ΔH° unknown.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1086 K: $Cp^\circ = 13.967 + 19.928x10^{-3}T - 1.710x10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 13.967x10^{-3}T + 9.964x10^{-6}T^{2} + 1.710x10^{2}T^{-1} - 5.624$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -41.829 + 5.611x10^{-3}T - 6.705x10^{-6}T^{2} + 423.950T^{-1}$
$\Delta Gf^\circ = -41.829 - 5.611x10^{-3}T\ln T + 6.705x10^{-6}T^{2} + 211.975T^{-1} + 64.758x10^{-3}T$
453.7-1086 K: $\Delta Hf^\circ = -40.510 - 9.683x10^{-3}T + 9.687x10^{-6}T^{2} + 466.850T^{-1}$
$\Delta Gf^\circ = -40.510 + 9.683x10^{-3}T\ln T - 9.687x10^{-6}T^{2} + 233.425T^{-1} - 24.376x10^{-3}T$

Source: Data from Osborne (378).

$LiNO_2(c,l)$
Lithium Nitrite
[Formation: $Li(c,l) + 0.5N_2(g) + O_2(g) = LiNO_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.100	21.000	21.000	0	-88.000	-70.754	51.863
300	15.200	21.130	21.030	.030	-88.001	-70.656	51.472
369	19.100	24.650	21.370	1.210	-87.968	-66.662	39.482
369	19.100	25.760	21.370	1.620	-87.558	-66.662	39.482
400	19.100	27.300	21.775	2.210	-87.500	-64.911	35.465
453.7	19.100	29.716	22.572	3.241	-87.413	-61.885	29.810
453.7	19.100	29.716	22.572	3.241	-88.130	-61.885	29.810
495	19.100	31.380	23.236	4.030	-88.090	-59.494	26.267
495	21.500	35.820	23.236	6.230	-85.890	-59.494	26.267
500	21.500	36.040	23.380	6.330	-85.881	-59.236	25.892
600	21.500	39.960	25.827	8.480	-85.555	-53.938	19.647
700	21.500	43.270	28.084	10.630	-85.247	-48.690	15.202
800	21.500	46.150	30.163	12.790	-84.948	-43.486	11.880
900	21.500	48.680	32.080	14.940	-84.682	-38.317	9.305
1000	21.500	50.950	33.860	17.090	-84.437	-33.184	7.252
1100	21.500	53.000	35.509	19.240	-84.208	-28.070	5.577
1200	21.500	54.870	37.045	21.390	-83.994	-22.976	4.184
1300	21.500	56.590	38.482	23.540	-83.792	-17.898	3.009
1400	21.500	58.180	39.830	25.690	-83.601	-12.832	2.003
1500	21.500	59.670	41.110	27.840	-83.419	-7.794	1.136

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 369 K, α - β transition point of $LiNO_2$; ΔH° = 0.410 kcal/mol.
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
495 K, melting point of $LiNO_2$; ΔH° = 2.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-369 K: $Cp° = -2.040 + 57.346\times10^{-3}T$
$H°-H°_{298} = -2.040\times10^{-3}T + 28.673\times10^{-6}T^2 - 1.941$
369-495 K: $Cp° = 19.120$
$H°-H°_{298} = 19.120\times10^{-3}T - 5.435$
495-1500 K: $Cp° = 21.500$
$H°-H°_{298} = 21.500\times10^{-3}T - 4.413$

Formation equations (kcal/mol):

298.15-369 K: $\Delta Hf° = -85.891 - 14.227\times10^{-3}T + 22.418\times10^{-6}T^2 + 41.750T^{-1}$
$\Delta Gf° = -85.891 + 14.227\times10^{-3}T\ln T - 22.418\times10^{-6}T^2 + 20.875T^{-1} - 23.844\times10^{-3}T$
369-453.7 K: $\Delta Hf° = -89.385 + 6.932\times10^{-3}T - 6.255\times10^{-6}T^2 + 41.750T^{-1}$
$\Delta Gf° = -89.385 - 6.932\times10^{-3}T\ln T + 6.255\times10^{-6}T^2 + 20.875T^{-1} + 100.117\times10^{-3}T$
453.7-495 K: $\Delta Hf° = -88.945 + 1.835\times10^{-3}T - 0.791\times10^{-6}T^2 + 56.050T^{-1}$
$\Delta Gf° = -88.945 - 1.835\times10^{-3}T\ln T + 0.791\times10^{-6}T^2 + 28.025T^{-1} + 70.405\times10^{-3}T$
495-1500 K: $\Delta Hf° = -87.923 + 4.215\times10^{-3}T - 0.791\times10^{-6}T^2 + 56.050T^{-1}$
$\Delta Gf° = -87.923 - 4.215\times10^{-3}T\ln T + 0.791\times10^{-6}T^2 + 28.025T^{-1} + 83.108\times10^{-3}T$

Source: Data from Gurvich (193) who estimated all except enthalpy of formation at 298 K.

$LiNO_3$(c,l)
Lithium Nitrate
[Formation: $Li(c,l) + 0.5N_2(g) + 1.5O_2(g) = LiNO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	20.210	21.500	21.500	0	-115.500	-91.097	66.775
300	20.304	21.625	21.502	.037	-115.500	-90.946	66.254
350	22.578	24.932	21.755	1.112	-115.427	-86.857	54.235
400	24.333	28.067	22.352	2.286	-115.285	-82.785	45.231
450	25.775	31.017	23.150	3.540	-115.091	-78.735	38.238
453.7	25.891	31.229	23.215	3.636	-115.074	-78.436	37.783
453.7	25.891	31.229	23.215	3.636	-115.791	-78.436	37.783
500	27.340	33.811	24.079	4.866	-115.572	-74.632	32.621
529.7*	28.555	35.421	24.670	5.695	-115.394	-72.205	29.791
529.7	33.606	46.673	24.670	11.655	-109.434	-72.205	29.791
550	33.606	47.937	25.506	12.337	-109.198	-70.783	28.126
600	33.606	50.861	27.498	14.018	-108.622	-67.316	24.519
650	33.606	53.551	29.400	15.698	-108.054	-63.898	21.484
700	33.606	56.041	31.215	17.378	-107.492	-60.522	18.896
750	33.606	58.360	32.949	19.058	-106.938	-57.189	16.665
800	33.606	60.529	34.605	20.739	-106.392	-53.889	14.722
850	33.606	62.566	36.191	22.419	-105.854	-50.624	13.016
900	33.606	64.487	37.710	24.099	-105.323	-47.390	11.508

*Data extrapolated above 520 K.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
529.7 K, melting point of $LiNO_3$ ΔH° = 5.960 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-529.7 K: $Cp° = 18.410 + 21.016\times10^{-3}T - 3.970\times10^{5}T^{-2}$
$H°-H°_{298} = 18.410\times10^{-3}T + 10.508\times10^{-6}T^{2} + 3.970\times10^{2}T^{-1} - 7.755$
529.7-900 K: $Cp° = 33.606$
$H°-H°_{298} = 33.606\times10^{-3}T - 6.146$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -118.029 + 2.607\times10^{-3}T + 4.001\times10^{-6}T^{2} + 416.150T^{-1}$
$\Delta Gf° = -118.029 - 2.607\times10^{-3}T\ln T - 4.001\times10^{-6}T^{2} + 208.075T^{-1} + 104.037\times10^{-3}T$
453.7-529.7 K: $\Delta Hf° = -117.589 - 2.491\times10^{-3}T + 9.465\times10^{-6}T^{2} + 430.450T^{-1}$
$\Delta Gf° = -117.589 + 2.491\times10^{-3}T\ln T - 9.465\times10^{-6}T^{2} + 215.225T^{-1} + 74.325\times10^{-3}T$
529.7-900 K: $\Delta Hf° = -115.981 + 12.705\times10^{-3}T - 1.043\times10^{-6}T^{2} + 33.450T^{-1}$
$\Delta Gf° = -115.981 - 12.705\times10^{-3}T\ln T + 1.043\times10^{-6}T^{2} + 16.725T^{-1} + 161.744\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (516). Enthalpy of fusion from Kleppa (274). Other data based on Ichikawa (212). Data extrapolated above 520 K.

LiOH(c,l)
Lithium Hydroxide
[Formation: $Li(c,l,g) + 0.5O_2(g) + 0.5H_2(g) = LiOH(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.853	10.235	10.235	0	-115.900	-104.921	76.908
300	11.893	10.308	10.235	.022	-115.902	-104.853	76.384
400	13.875	14.024	10.727	1.319	-115.928	-101.161	55.271
453.7	14.593	15.823	11.225	2.086	-115.909	-99.182	47.776
453.7	14.593	15.823	11.225	2.086	-116.626	-99.182	47.776
500	15.212	17.271	11.719	2.776	-116.604	-97.400	42.573
600	16.302	20.143	12.888	4.353	-116.468	-93.570	34.082
700	17.275	22.730	14.113	6.032	-116.229	-89.773	28.028
744.3	17.678	23.818	14.685	6.798	-116.101	-88.122	25.875
744.3	20.814	30.529	14.685	11.793	-111.106	-88.122	25.875
800	20.814	32.031	15.840	12.953	-110.751	-86.415	23.607
900*	20.814	34.483	17.779	15.034	-110.124	-83.412	20.255
1000	20.814	36.676	19.561	17.115	-109.506	-80.477	17.588
1100	20.814	38.660	21.208	19.197	-108.894	-77.603	15.418
1200	20.814	40.471	22.739	21.278	-108.293	-74.786	13.620
1300	20.814	42.137	24.168	23.360	-107.698	-72.018	12.107
1400	20.814	43.679	25.507	25.441	-107.112	-69.295	10.817
1500	20.814	45.115	26.767	27.522	-106.533	-66.615	9.706
1600	20.814	46.459	27.956	29.604	-105.959	-63.972	8.738
1638	20.814	46.948	28.391	30.395	-105.742	-62.978	8.403
1638	20.814	46.948	28.391	30.395	-140.902	-62.978	8.403
1700	20.814	47.720	29.082	31.685	-140.440	-60.033	7.718
1800	20.814	48.910	30.151	33.767	-139.698	-55.325	6.717
1900	20.814	50.036	31.169	35.848	-138.965	-50.660	5.827

*Heat capacities extrapolated above 873 K.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
744.3 K, melting point of LiOH; ΔH° = 4.995 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-744.3 K: $Cp° = 12.474 + 7.496\times10^{-3}T - 2.539\times10^{5}T^{-2}$
$H°-H°_{298} = 12.474\times10^{-3}T + 3.748\times10^{-6}T^{2} + 2.539\times10^{2}T^{-1} - 4.904$
744.3-1900 K: $Cp° = 20.814$
$H°-H°_{298} = 20.814\times10^{-3}T - 3.699$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -117.961 + 3.932\times10^{-3}T - 2.171\times10^{-6}T^{2} + 322.550T^{-1}$
$\Delta Gf° = -117.961 - 3.932\times10^{-3}T\ln T + 2.171\times10^{-6}T^{2} + 161.275T^{-1} + 63.680\times10^{-3}T$
453.7-744.3 K: $\Delta Hf° = -117.521 - 1.166\times10^{-3}T + 3.293\times10^{-6}T^{2} + 336.850T^{-1}$
$\Delta Gf° = -117.521 + 1.166\times10^{-3}T\ln T - 3.293\times10^{-6}T^{2} + 168.425T^{-1} + 33.968\times10^{-3}T$
744.3-1638 K: $\Delta Hf° = -116.316 + 7.174\times10^{-3}T - 0.455\times10^{-6}T^{2} + 82.950T^{-1}$
$\Delta Gf° = -116.316 - 7.174\times10^{-3}T\ln T + 0.455\times10^{-6}T^{2} + 41.475T^{-1} + 84.936\times10^{-3}T$
1638-1900 K: $\Delta Hf° = -153.783 + 8.760\times10^{-3}T - 0.439\times10^{-6}T^{2} - 464.950T^{-1}$
$\Delta Gf° = -153.783 - 8.760\times10^{-3}T\ln T + 0.439\times10^{-6}T^{2} - 232.475T^{-1} + 119.676\times10^{-3}T$

Source: Data from Chase (81) who extrapolated heat capacities above 873 K.

LiOH(g)
Lithium Hydroxide (ideal gas)

[Formation: $Li(c,l,g) + 0.5O_2(g) + 0.5H_2(g) = LiOH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	11.025	50.321	50.321	0	-56.000	-56.972	41.761
300	11.042	50.389	50.322	.020	-56.004	-56.979	41.509
400	11.731	53.671	50.764	1.163	-56.184	-57.275	31.293
453.7	11.938	55.164	51.197	1.800	-56.295	-57.417	27.658
453.7	11.938	55.164	51.197	1.800	-57.012	-57.417	27.658
500	12.116	56.333	51.619	2.357	-57.123	-57.450	25.111
600	12.361	58.565	52.597	3.581	-57.340	-57.495	20.942
700	12.543	60.485	53.589	4.827	-57.534	-57.506	17.954
800	12.698	62.170	54.559	6.089	-57.715	-57.490	15.705
900	12.843	63.674	55.490	7.366	-57.892	-57.451	13.951
1000	12.983	65.035	56.378	8.657	-58.064	-57.395	12.543
1100	13.119	66.279	57.222	9.963	-58.228	-57.318	11.388
1200	13.248	67.426	58.025	11.281	-58.390	-57.229	10.423
1300	13.371	68.491	58.789	12.612	-58.546	-57.126	9.604
1400	13.486	69.486	59.518	13.955	-58.698	-57.010	8.900
1500	13.593	70.420	60.214	15.309	-58.846	-56.885	8.288
1600	13.691	71.301	60.880	16.673	-58.990	-56.750	7.752
1638	13.725	71.623	61.126	17.194	-59.043	-56.697	7.565
1638	13.725	71.623	61.126	17.194	-94.203	-56.697	7.565
1700	13.781	72.134	61.518	18.047	-94.178	-55.275	7.106
1800	13.864	72.924	62.130	19.429	-94.136	-52.988	6.434
1900	13.939	73.675	62.718	20.819	-94.094	-50.703	5.832
2000	14.008	74.392	63.284	22.217	-94.050	-48.419	5.291

Phase changes: 453.7 K, melting point of Li; $\Delta H° = 0.717$ kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; $\Delta H° = 35.160$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.064 + 1.042\times10^{-3}T - 1.199\times10^{5}T^{-2}$
$H°-H°_{298} = 12.064\times10^{-3}T + 0.521\times10^{-6}T^{2} + 1.199\times10^{2}T^{-1} - 4.045$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -57.203 + 3.522\times10^{-3}T - 5.398\times10^{-6}T^{2} + 188.550T^{-1}$
$\Delta Gf° = -57.203 - 3.522\times10^{-3}T\ln T + 5.398\times10^{-6}T^{2} + 94.275T^{-1} + 18.170\times10^{-3}T$
453.7-1638 K: $\Delta Hf° = -56.763 - 1.576\times10^{-3}T + 0.066\times10^{-6}T^{2} + 202.850T^{-1}$
$\Delta Gf° = -56.763 + 1.576\times10^{-3}T\ln T - 0.066\times10^{-6}T^{2} + 101.425T^{-1} - 11.542\times10^{-3}T$
1638-2000 K: $\Delta Hf° = -94.229 + 0.010\times10^{-3}T + 0.082\times10^{-6}T^{2} - 345.050T^{-1}$
$\Delta Gf° = -94.229 - 0.010\times10^{-3}T\ln T - 0.082\times10^{-6}T^{2} - 172.525T^{-1} + 23.198\times10^{-3}T$

Source: Data from Chase (81) who estimated some molecular constants.

$(LiOH)_2(g)$
Dimeric Lithium Hydroxide (ideal gas)
[Formation: $2Li(s,l,g) + O_2(g) + H_2(g) = (LiOH)_2(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	17.022	64.453	64.453	0	-170.000	-161.155	118.128
300	17.075	64.558	64.453	.032	-170.016	-161.100	117.360
400	19.542	69.825	65.155	1.868	-170.826	-158.002	86.327
453.7	20.548	72.357	65.858	2.949	-171.242	-156.258	75.269
453.7	20.548	72.357	65.858	2.949	-172.676	-156.258	75.269
500	21.415	74.396	66.556	3.920	-173.040	-154.560	67.557
600	22.835	78.432	68.205	6.136	-173.705	-150.798	54.927
700	23.931	82.038	69.929	8.476	-174.245	-146.938	45.876
800	24.808	85.293	71.649	10.915	-174.694	-143.006	39.067
900	25.535	88.258	73.332	13.433	-175.083	-139.021	33.758
1000	26.154	90.981	74.963	16.018	-175.423	-134.996	29.503
1100	26.693	93.500	76.535	18.661	-175.721	-130.938	26.015
1200	27.166	95.843	78.047	21.355	-175.987	-126.854	23.103
1300	27.584	98.034	79.501	24.093	-176.223	-122.750	20.636
1400	27.955	100.092	80.899	26.870	-176.436	-118.629	18.519
1500	28.286	102.032	82.244	29.682	-176.627	-114.494	16.682
1600	28.581	103.867	83.538	32.526	-176.799	-110.345	15.072
1638	28.681	104.539	84.018	33.614	-176.860	-108.767	14.512
1638	28.681	104.539	84.018	33.614	-247.180	-108.767	14.512
1700	28.844	105.608	84.786	35.397	-247.053	-103.525	13.309
1800	29.080	107.264	85.990	38.294	-246.835	-95.090	11.545
1900	29.291	108.842	87.151	41.212	-246.613	-86.667	9.969
2000	29.480	110.349	88.273	44.151	-246.384	-78.252	8.551

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.225 + 4.970 \times 10^{-3}T - 5.054 \times 10^{5}T^{-2}$

$H° - H°_{298} = 21.225 \times 10^{-3}T + 2.485 \times 10^{-6}T^{2} + 5.054 \times 10^{2}T^{-1} - 8.244$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -172.559 + 4.141 \times 10^{-3}T - 9.353 \times 10^{-6}T^{2} + 642.700T^{-1}$

$\Delta Gf° = -172.559 - 4.141 \times 10^{-3}T\ln T + 9.353 \times 10^{-6}T^{2} + 321.350T^{-1} + 55.440 \times 10^{-3}T$

453.7-1638 K: $\Delta Hf° = -171.679 - 6.055 \times 10^{-3}T + 1.575 \times 10^{-6}T^{2} + 671.300T^{-1}$

$\Delta Gf° = -171.679 + 6.055 \times 10^{-3}T\ln T - 1.575 \times 10^{-6}T^{2} + 335.650T^{-1} - 3.984 \times 10^{-3}T$

1638-2000 K: $\Delta Hf° = -246.612 - 2.883 \times 10^{-3}T + 1.607 \times 10^{-6}T^{2} - 424.500T^{-1}$

$\Delta Gf° = -246.612 + 2.883 \times 10^{-3}T\ln T - 1.607 \times 10^{-6}T^{2} - 212.250T^{-1} + 65.496 \times 10^{-3}T$

Source: Data from Chase (81) who estimated all except enthalpy of formation at 298 K.

$LiPO_3(c)$
Lithium Metaphosphate
[Formation: $Li(c,l) + P(c,l,1/4P_4(g)) + 1.5O_2(g) = LiPO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$ΔHf°$	$ΔGf°$	
298.15*	20.810	17.330	17.330	0	-300.000	-278.250	203.960
300	20.900	17.460	17.330	.040	-300.001	-278.114	202.603
317.3	21.505	18.649	17.367	.407	-300.019	-276.850	190.686
317.3	21.505	18.649	17.367	.407	-300.176	-276.850	190.686
400	24.400	24.010	18.210	2.320	-300.184	-270.772	147.941
453.7	25.512	27.164	19.083	3.667	-300.125	-266.827	128.530
453.7	25.512	27.164	19.083	3.667	-300.842	-266.827	128.530
500	26.470	29.690	19.950	4.870	-300.777	-263.356	115.111
550	27.220	32.249	20.939	6.220	-300.662	-259.626	103.164
550	27.220	32.249	20.939	6.220	-303.570	-259.626	103.164
600	27.970	34.650	21.983	7.600	-303.348	-255.640	93.116
700	29.210	39.060	24.117	10.460	-302.828	-247.731	77.344
800	30.310	43.030	26.230	13.440	-302.215	-239.897	65.536
900	31.330	46.660	28.304	16.520	-301.529	-232.150	56.373

*Data except enthalpy of formation at 298 K estimated.

Phase changes:
317.3 K, melting point of P; $ΔH° = 0.157$ kcal/mol.
453.7 K, melting point of Li; $ΔH° = 0.717$ kcal/mol.
550 K, boiling point of P to $P_4(g)$; $ΔH° = 2.908$ kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K:
$Cp° = 24.480 + 8.360\times10^{-3}T - 5.480\times10^{5}T^{-2}$
$H°-H°_{298} = 24.480\times10^{-3}T + 4.180\times10^{-6}T^{2} + 5.480\times10^{2}T^{-1} - 9.508$

Formation equations (kcal/mol):

298.15-317.3 K:
$ΔHf° = -303.851 + 8.137\times10^{-3}T - 5.218\times10^{-6}T^{2} + 563.200T^{-1}$
$ΔGf° = -303.851 - 8.137\times10^{-3}T\ln T + 5.218\times10^{-6}T^{2} + 281.600T^{-1} + 127.506\times10^{-3}T$

317.3-453.7 K:
$ΔHf° = -303.538 + 5.644\times10^{-3}T - 2.032\times10^{-6}T^{2} + 563.200T^{-1}$
$ΔGf° = -303.538 - 5.644\times10^{-3}T\ln T + 2.032\times10^{-6}T^{2} + 281.600T^{-1} + 113.170\times10^{-3}T$

453.7-550 K:
$ΔHf° = -303.098 + 0.546\times10^{-3}T + 3.432\times10^{-6}T^{2} + 577.500T^{-1}$
$ΔGf° = -303.098 - 0.546\times10^{-3}T\ln T - 3.432\times10^{-6}T^{2} + 288.750T^{-1} + 83.458\times10^{-3}T$

550-900 K:
$ΔHf° = -306.558 + 1.884\times10^{-3}T + 3.428\times10^{-6}T^{2} + 477.200T^{-1}$
$ΔGf° = -306.558 - 1.884\times10^{-3}T\ln T - 3.428\times10^{-6}T^{2} + 238.600T^{-1} + 98.356\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data are those estimated by Beglov (25).

$Li_4P_2O_7(c)$
Lithium Pyrophosphate
[Formation: $4Li(c,l) + 2P(c,l,1/4P_4(g)) + 3.5O_2(g) = Li_4P_2O_7(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^\circ_{298})/T$	$H°-H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	58.730	42.600	42.600	0	-802.000	-749.414	549.328
300	58.790	42.960	42.600	.110	-802.002	-749.087	545.703
317.3	59.390	46.273	42.704	1.132	-802.016	-746.033	513.846
317.3	59.390	46.273	42.704	1.132	-802.330	-746.033	513.846
400	62.260	60.350	44.950	6.160	-802.473	-731.343	399.582
453.7	64.123	68.311	47.253	9.554	-802.581	-721.796	347.689
453.7	64.123	68.311	47.253	9.554	-805.449	-721.796	347.689
500	65.730	74.620	49.500	12.560	-805.561	-713.244	311.755
550	67.465	80.964	52.067	15.893	-805.601	-704.033	279.753
550	67.465	80.964	52.067	15.893	-811.417	-704.033	279.753
600	69.200	86.910	54.727	19.310	-811.218	-694.278	252.887
700	72.670	97.840	60.126	26.400	-810.594	-674.841	210.692
800	76.140	107.770	65.470	33.840	-809.671	-655.511	179.075
900	79.610	116.930	70.674	41.630	-808.458	-636.299	154.512

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp° = 48.380 + 34.700\times10^{-3}T$
$H°-H^\circ_{298} = 48.380\times10^{-3}T + 17.350\times10^{-6}T^2 - 15.967$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -804.050 + 8.681\times10^{-3}T - 12.613\times10^{-6}T^2 + 173.800T^{-1}$
$\Delta Gf° = -804.050 - 8.681\times10^{-3}T\ln T + 12.613\times10^{-6}T^2 + 86.900T^{-1} + 227.972\times10^{-3}T$
317.3-453.7 K: $\Delta Hf° = -803.423 + 3.695\times10^{-3}T - 6.243\times10^{-6}T^2 + 173.800T^{-1}$
$\Delta Gf° = -803.423 - 3.695\times10^{-3}T\ln T + 6.243\times10^{-6}T^2 + 86.900T^{-1} + 199.300\times10^{-3}T$
453.7-550 K: $\Delta Hf° = -801.665 - 16.697\times10^{-3}T + 15.613\times10^{-6}T^2 + 231.000T^{-1}$
$\Delta Gf° = -801.665 + 16.697\times10^{-3}T\ln T - 15.613\times10^{-6}T^2 + 115.500T^{-1} + 80.453\times10^{-3}T$
550-900 K: $\Delta Hf° = -808.585 - 14.021\times10^{-3}T + 15.605\times10^{-6}T^2 + 30.400T^{-1}$
$\Delta Gf° = -808.585 + 14.021\times10^{-3}T\ln T - 15.605\times10^{-6}T^2 + 15.200T^{-1} + 110.249\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data are those estimated by Beglov (25).

$Li_2SO_4(c,l)$
Lithium Sulfate
[Reaction: $2Li(c,l,g) + 0.5S_2(g) + 2O_2(g) = Li_2SO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15	28.109	27.234	27.234	0	-358.655	-325.281	238.434
300	28.209	27.408	27.235	.052	-358.658	-325.074	236.813
400	33.280	36.252	28.407	3.138	-358.633	-313.874	171.490
453.7	35.235	40.570	29.593	4.981	-358.522	-307.874	148.303
453.7	35.235	40.570	29.593	4.981	-359.956	-307.874	148.303
500	36.920	44.076	30.774	6.651	-359.831	-302.561	132.247
600	40.215	51.099	33.584	10.509	-359.333	-291.146	106.049
700	43.450	57.544	36.554	14.693	-358.536	-279.844	87.370
800	46.520	63.531	39.555	19.181	-357.464	-268.673	73.397
848	48.454	66.296	40.991	21.459	-356.837	-263.363	67.874
848	51.000	74.315	40.991	28.259	-350.037	-263.363	67.874
900	51.000	77.351	43.005	30.911	-349.183	-258.075	62.668
1000	51.000	82.724	46.713	36.011	-347.561	-248.038	54.208
1100	51.000	87.585	50.211	41.111	-345.962	-238.162	47.318
1132	51.000	89.047	51.288	42.743	-345.455	-235.033	45.376
1132	49.000	90.858	51.288	44.793	-343.405	-235.033	45.376
1200	49.000	93.717	53.613	48.125	-342.471	-228.552	41.625
1300	49.000	97.639	56.851	53.025	-341.110	-219.115	36.836
1400	49.000	101.270	59.895	57.925	-339.767	-209.781	32.748
1500	49.000	104.651	62.768	62.825	-338.434	-200.545	29.219
1600	49.000	107.813	65.485	67.725	-337.116	-191.393	26.143
1638	49.000	108.963	66.480	69.587	-336.617	-187.939	25.075
1638	49.000	108.963	66.480	69.587	-406.937	-187.939	25.075
1700	49.000	110.784	68.063	72.625	-405.905	-179.665	23.097
1800	49.000	113.584	70.515	77.525	-404.247	-166.402	20.204
1900	49.000	116.234	72.852	82.425	-402.607	-153.237	17.626
2000	49.000	118.747	75.085	87.325	-400.979	-140.151	15.315

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
848 K, α - β transition point of Li_2SO_4; ΔH° = 6.800 kcal/mol.
1132 K, melting point of Li_2SO_4; ΔH° = 2.050 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-848 K: $Cp^\circ = 24.519 + 28.288\times10^{-3}T - 4.306\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 24.519\times10^{-3}T + 14.144\times10^{-6}T^{2} + 4.306\times10^{2}T^{-1} - 10.012$
848-1132 K: $Cp^\circ = 51.000$
$H^\circ - H^\circ_{298} = 51.000\times10^{-3}T - 14.989$
1132-2000 K: $Cp^\circ = 49.000$
$H^\circ - H^\circ_{298} = 49.000\times10^{-3}T - 10.675$

Reaction equations (kcal/mol):

298.15-453.7 K: $\Delta Hr^\circ = -361.164 + 2.489\times10^{-3}T + 2.062\times10^{-6}T^{2} + 472.050T^{-1}$
$\Delta Gr^\circ = -361.164 - 2.489\times10^{-3}T\ln T - 2.062\times10^{-6}T^{2} + 236.025T^{-1} + 132.495\times10^{-3}T$
453.7-848 K: $\Delta Hr^\circ = -360.284 - 7.707\times10^{-3}T + 12.990\times10^{-6}T^{2} + 500.650T^{-1}$
$\Delta Gr^\circ = -360.284 + 7.707\times10^{-3}T\ln T - 12.990\times10^{-6}T^{2} + 250.325T^{-1} + 73.072\times10^{-3}T$
848-1132 K: $\Delta Hr^\circ = -365.262 + 18.774\times10^{-3}T - 1.154\times10^{-6}T^{2} + 70.050T^{-1}$
$\Delta Gr^\circ = -365.262 - 18.774\times10^{-3}T\ln T + 1.154\times10^{-6}T^{2} + 35.025T^{-1} + 245.805\times10^{-3}T$
1132-1638 K: $\Delta Hr^\circ = -360.948 + 16.774\times10^{-3}T - 1.154\times10^{-6}T^{2} + 70.050T^{-1}$
$\Delta Gr^\circ = -360.948 - 16.774\times10^{-3}T\ln T + 1.154\times10^{-6}T^{2} + 35.025T^{-1} + 227.931\times10^{-3}T$
1638-2000 K: $\Delta Hr^\circ = -435.880 + 19.946\times10^{-3}T - 1.122\times10^{-6}T^{2} - 1025.750T^{-1}$
$\Delta Gr^\circ = -435.880 - 19.946\times10^{-3}T\ln T + 1.122\times10^{-6}T^{2} - 512.875T^{-1} + 297.410\times10^{-3}T$

Source: Data from JANAF (128).

$Li_2SO_4(g)$
Lithium Sulfate (ideal gas)
[Reaction: $2Li(c,l,g) + 0.5S_2(g) + 2O_2(g) = Li_2SO_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	24.332	77.130	77.130	0	-264.355	-245.857	180.216
300	24.415	77.281	77.131	.045	-264.365	-245.743	179.021
400	28.128	84.847	78.137	2.684	-264.787	-239.466	130.836
453.7	29.480	88.491	79.147	4.239	-264.963	-236.057	113.709
453.7	29.480	88.491	79.147	4.239	-266.397	-236.057	113.709
500	30.645	91.412	80.150	5.631	-266.552	-232.949	101.821
600	32.363	97.161	82.516	8.787	-266.755	-226.206	82.394
700	33.561	102.245	84.979	12.086	-266.843	-219.441	68.512
800	34.416	106.785	87.426	15.487	-266.858	-212.670	58.098
900	35.043	110.877	89.808	18.962	-266.832	-205.897	49.998
1000	35.514	114.595	92.104	22.491	-266.781	-199.130	43.519
1100	35.874	117.997	94.305	26.061	-266.712	-192.366	38.219
1200	36.156	121.131	96.412	29.663	-266.634	-185.611	33.804
1300	36.380	124.035	98.427	33.290	-266.545	-178.865	30.070
1400	36.561	126.737	100.353	36.938	-266.453	-172.121	26.869
1500	36.709	129.265	102.197	40.602	-266.358	-165.389	24.097
1600	36.831	131.638	103.964	44.279	-266.262	-158.659	21.672
1638	36.870	132.503	104.616	45.679	-266.225	-156.105	20.828
1638	36.870	132.503	104.616	45.679	-336.545	-156.105	20.828
1700	36.934	133.874	105.658	47.967	-336.264	-149.276	19.191
1800	37.020	135.988	107.285	51.665	-335.808	-138.289	16.790
1900	37.094	137.991	108.848	55.371	-335.361	-127.329	14.646
2000	37.157	139.896	110.354	59.083	-334.922	-116.391	12.719

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 33.282 + 2.556\times10^{-3}T - 8.634\times10^{5}T^{-2}$
$H° - H°_{298} = 33.282\times10^{-3}T + 1.278\times10^{-6}T^{2} + 8.634\times10^{2}T^{-1} - 12.932$

Reaction equations (kcal/mol):

298.15-453.7 K: $\Delta Hr° = -269.784 + 11.253\times10^{-3}T - 10.804\times10^{-6}T^{2} + 904.850T^{-1}$
$\Delta Gr° = -269.784 - 11.253\times10^{-3}T\ln T + 10.804\times10^{-6}T^{2} + 452.425T^{-1} + 136.053\times10^{-3}T$
453.7-1638 K: $\Delta Hr° = -268.905 + 1.056\times10^{-3}T + 0.124\times10^{-6}T^{2} + 933.450T^{-1}$
$\Delta Gr° = -268.905 - 1.056\times10^{-3}T\ln T - 0.124\times10^{-6}T^{2} + 466.725T^{-1} + 76.629\times10^{-3}T$
1638-2000 K: $\Delta Hr° = -343.837 + 4.229\times10^{-3}T + 0.156\times10^{-6}T^{2} - 162.350T^{-1}$
$\Delta Gr° = -343.837 - 4.229\times10^{-3}T\ln T - 0.156\times10^{-6}T^{2} - 81.175T^{-1} + 146.109\times10^{-3}T$

Source: Data from JANAF (128).

$Li_2SO_4 \cdot H_2O(c)$
Lithium Sulfate Monohydrate
[Reaction: $2Li(c,l) + 0.5S_2(g) + 2.5O_2(g) + H_2(g) = Li_2SO_4 \cdot H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	36.100	34.995	34.995	0	-429.885	-382.215	280.168
300*	36.248	35.219	34.996	.067	-429.893	-381.919	278.224
350	39.772	41.083	35.452	1.971	-430.013	-373.912	233.478
400	42.384	46.574	36.502	4.029	-430.040	-365.893	199.912
450	44.084	51.674	37.910	6.194	-430.017	-357.880	173.808
453.7	44.142	52.035	38.023	6.357	-430.014	-357.287	172.105
453.7	44.142	52.035	38.023	6.357	-431.448	-357.287	172.105
500	44.872	56.367	39.523	8.422	-431.423	-349.715	152.858
550	44.748	60.645	41.250	10.667	-431.392	-341.544	135.715

*Data above 298 K estimated.

Phase change: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 52.514 - 4.806 \times 10^{-3}T - 13.317 \times 10^{5}T^{-2}$

$H° - H°_{298} = 52.514 \times 10^{-3}T - 2.403 \times 10^{-6}T^{2} + 13.317 \times 10^{2}T^{-1} - 19.910$

Reaction equations (kcal/mol):

298.15-453.7 K: $\Delta Hr° = -439.209 + 20.413 \times 10^{-3}T - 15.155 \times 10^{-6}T^{2} + 1367.050T^{-1}$

$\Delta Gr° = -439.209 - 20.413 \times 10^{-3}T\ln T + 15.155 \times 10^{-6}T^{2} + 683.525T^{-1} + 295.259 \times 10^{-3}T$

453.7-550 K: $\Delta Hr° = -438.330 + 10.218 \times 10^{-3}T - 4.227 \times 10^{-6}T^{2} + 1395.650T^{-1}$

$\Delta Gr° = -438.330 - 10.218 \times 10^{-3}T\ln T + 4.227 \times 10^{-6}T^{2} + 697.825T^{-1} + 235.836 \times 10^{-3}T$

Source: Data from DeKock (113) who estimated all above 298 K.

Li_2SiO_3(c)
Lithium Silicate
[Formation: $2Li(c,l) + Si(c) + 1.5O_2(g) = Li_2SiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	23.880	19.080	19.080	0	-393.800	-372.084	272.741
300	24.000	19.230	19.083	.044	-393.806	-371.950	270.962
400	28.560	26.830	20.087	2.697	-393.967	-364.634	199.224
453.7	30.037	30.539	21.108	4.279	-393.991	-360.698	173.748
453.7	30.037	30.539	21.108	4.279	-395.425	-360.698	173.748
500	31.310	33.520	22.122	5.699	-395.444	-357.148	156.107
600	33.240	39.410	24.523	8.932	-395.341	-349.497	127.303
700	34.720	44.650	27.029	12.335	-395.096	-341.874	106.737
800	35.920	49.360	29.529	15.865	-394.753	-334.292	91.323
900	36.930	53.650	31.972	19.510	-394.330	-326.756	79.346
1000	37.800	57.590	34.340	23.250	-393.839	-319.266	69.775
1100	38.580	61.230	36.625	27.065	-393.296	-311.846	61.957
1200	39.270	64.620	38.820	30.960	-392.693	-304.471	55.451
1300	39.880	67.780	40.918	34.920	-392.039	-297.134	49.952
1400	40.410	70.760	42.949	38.935	-391.346	-289.861	45.249
1475	40.740	72.880	44.419	41.980	-390.801	-284.453	42.147

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1475 K, melting point of Li_2SiO_3; ΔH° unknown.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1475 K: $Cp° = 30.687 + 7.802 \times 10^{-3}T - 8.119 \times 10^{5}T^{-2}$

$H°-H°_{298} = 30.687 \times 10^{-3}T + 3.901 \times 10^{-6}T^{2} + 8.119 \times 10^{2}T^{-1} - 12.219$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -399.010 + 10.765 \times 10^{-3}T - 8.121 \times 10^{-6}T^{2} + 811.600T^{-1}$

$\Delta Gf° = -399.010 - 10.765 \times 10^{-3}T\ln T + 8.121 \times 10^{-6}T^{2} + 405.800T^{-1} + 144.658 \times 10^{-3}T$

453.7-1475 K: $\Delta Hf° = -398.130 + 0.569 \times 10^{-3}T + 2.808 \times 10^{-6}T^{2} + 840.200T^{-1}$

$\Delta Gf° = -398.130 - 0.569 \times 10^{-3}T\ln T - 2.808 \times 10^{-6}T^{2} + 420.100T^{-1} + 85.235 \times 10^{-3}T$

Source: Data from Bennington (35).

$Li_2Si_2O_5(c)$
Lithium Disilicate
[Formation: $2Li(c,l) + 2Si(c) + 2.5O_2(g) = Li_2Si_2O_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	34.590	29.200	29.200	0	-611.800	-577.149	423.056
300	34.730	29.410	29.200	.064	-611.808	-576.933	420.290
400	41.230	40.370	30.645	3.890	-612.013	-565.268	308.844
453.7	43.512	45.726	32.112	6.177	-612.011	-558.991	269.266
453.7	43.512	45.726	32.112	6.177	-613.445	-558.991	269.266
500	45.480	50.050	33.576	8.237	-613.422	-553.431	241.901
600	48.570	58.630	37.055	12.945	-613.172	-541.457	197.223
700	50.920	66.300	40.693	17.925	-612.719	-529.539	165.327
800	52.760	73.230	44.336	23.115	-612.117	-517.697	141.426
900	54.260	79.530	47.897	28.470	-611.419	-505.929	122.855
1000	55.540	85.320	51.360	33.960	-610.633	-494.240	108.015
1100	56.710	90.670	54.693	39.575	-609.766	-482.655	95.893
1200	57.880	95.650	57.900	45.300	-608.825	-471.141	85.805
1215	58.060	96.370	58.370	46.170	-608.675	-469.421	84.437
1215	59.500	96.580	58.370	46.425	-608.420	-469.421	84.437
1300	59.500	100.600	61.000	51.480	-607.456	-459.729	77.286
1307	59.500	100.900	61.191	51.900	-607.375	-458.905	76.735

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1215 K, α - β transition point of $Li_2Si_2O_5$; ΔH° = 0.255 kcal/mol.
1307 K, melting point of $Li_2Si_2O_5$; ΔH° unknown.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1215 K: $Cp° = 42.977 + 13.812 \times 10^{-3}T - 11.120 \times 10^{5}T^{-2}$
$H°- H°_{298} = 42.977 \times 10^{-3}T + 6.906 \times 10^{-6}T^{2} + 11.120 \times 10^{2}T^{-1} - 17.157$
1215-1307 K: $Cp° = 59.501$
$H°- H°_{298} = 59.501 \times 10^{-3}T - 25.869$

Formation equations (kcal/mol):

298.15-453.7 K: $ΔHf° = -617.541 + 10.146 \times 10^{-3}T - 5.970 \times 10^{-6}T^{2} + 968.000T^{-1}$
$ΔGf° = -617.541 - 10.146 \times 10^{-3}T\ln T + 5.970 \times 10^{-6}T^{2} + 484.000T^{-1} + 186.059 \times 10^{-3}T$
453.7-1215 K: $ΔHf° = -616.662 - 0.050 \times 10^{-3}T + 4.958 \times 10^{-6}T^{2} + 996.600T^{-1}$
$ΔGf° = -616.662 + 0.050 \times 10^{-3}T\ln T - 4.958 \times 10^{-6}T^{2} + 498.300T^{-1} + 126.636 \times 10^{-3}T$
1215-1307 K: $ΔHf° = -625.373 + 16.474 \times 10^{-3}T - 1.948 \times 10^{-6}T^{2} - 115.400T^{-1}$
$ΔGf° = -625.373 - 16.474 \times 10^{-3}T\ln T + 1.948 \times 10^{-6}T^{2} - 57.700T^{-1} + 243.154 \times 10^{-3}T$

Source: Data from Bennington (35).

$Li_2TiO_3(c,l)$
Lithium Titanate
[Formation: $2Li(c,l,g) + Ti(c,l) + 1.5O_2(g) = Li_2TiO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	26.530	21.930	21.930	0	-399.300	-377.593	276.780
300	26.636	22.094	21.931	.049	-399.303	-377.458	274.974
400	30.513	30.358	23.031	2.931	-399.344	-370.162	202.245
453.7	31.594	34.288	24.132	4.608	-399.327	-366.251	176.423
453.7	31.594	34.288	24.132	4.608	-400.761	-366.251	176.423
500	32.526	37.403	25.219	6.092	-400.759	-362.725	158.545
600	33.801	43.454	27.767	9.412	-400.661	-355.125	129.353
700	34.726	48.737	30.393	12.841	-400.488	-347.544	108.507
800	35.466	53.424	32.985	16.351	-400.272	-339.999	92.882
900	36.098	57.638	35.494	19.930	-400.034	-332.476	80.735
1000	36.663	61.471	37.902	23.569	-399.774	-324.982	71.024
1100	37.184	64.990	40.206	27.262	-399.499	-317.521	63.085
1156	37.459	66.844	41.453	29.352	-399.338	-313.350	59.240
1156	37.459	66.844	41.453	29.352	-400.355	-313.350	59.240
1200	37.675	68.247	42.410	31.005	-400.178	-310.042	56.466
1300	38.145	71.281	44.515	34.796	-399.764	-302.547	50.862
1400	38.600	74.125	46.530	38.633	-399.335	-295.086	46.064
1485	38.977	76.411	48.175	41.930	-398.952	-288.767	42.498
1485	43.060	78.185	48.175	44.565	-396.317	-288.767	42.498
1500	43.060	78.618	48.477	45.211	-396.188	-287.681	41.915
1600	43.060	81.397	50.449	49.517	-395.341	-280.475	38.311
1638	43.060	82.408	51.179	51.153	-395.026	-277.751	37.058
1638	43.060	82.408	51.179	51.153	-465.346	-277.751	37.058
1700	43.060	84.008	52.347	53.823	-464.620	-270.660	34.795
1800	43.060	86.469	54.175	58.129	-463.476	-259.284	31.481
1820	43.060	86.945	54.533	58.990	-463.253	-257.017	30.863
1820	45.300	101.505	54.533	85.490	-436.753	-257.107	30.863
1900	45.300	103.454	56.552	89.114	-435.700	-249.140	28.657
1945	45.300	104.514	57.649	91.152	-435.123	-244.730	27.499
1945	45.300	104.514	57.649	91.152	-438.423	-244.730	27.499
2000	45.300	105.777	58.955	93.644	-437.830	-239.257	26.145

Phase changes:
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1485 K, α - β transition point of Li_2TiO_3; ΔH° = 2.635 kcal/mol.
1638 K, boiling point of Li to ideal monatomic gas; ΔH° = 35.160 kcal/mol.
1820 K, melting point of Li_2TiO_3; ΔH° = 26.500 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1485 K: $Cp° = 33.419 + 3.962x10^{-3}T - 7.185x10^{5}T^{-2}$
$H°- H°_{298} = 33.419x10^{-3}T + 1.981x10^{-6}T^{2} + 7.185x10^{2}T^{-1} - 12.550$
1485-1820 K: $Cp° = 43.060$
$H°- H°_{298} = 43.060x10^{-3}T - 19.379$
1820-2000 K: $Cp° = 45.300$
$H°- H°_{298} = 45.300x10^{-3}T + 3.044$

Formation equations (kcal/mol):

298.15-453.7 K: $ΔHf° = -405.113 + 13.699x10^{-3}T - 10.813x10^{-6}T^{2} + 801.900T^{-1}$
$ΔGf° = -405.113 - 13.699x10^{-3}TlnT + 10.813x10^{-6}T^{2} + 400.950T^{-1} + 162.619x10^{-3}T$
453.7-1156 K: $ΔHf° = -404.233 + 3.503x10^{-3}T + 0.115x10^{-6}T^{2} + 830.500T^{-1}$
$ΔGf° = -404.233 - 3.503x10^{-3}TlnT - 0.115x10^{-6}T^{2} + 415.250T^{-1} + 103.196x10^{-3}T$
1156-1485 K: $ΔHf° = -408.270 + 5.903x10^{-3}T - 0.208x10^{-6}T^{2} + 1613.400T^{-1}$
$ΔGf° = -408.270 - 5.903x10^{-3}TlnT + 0.208x10^{-6}T^{2} + 806.700T^{-1} + 122.948x10^{-3}T$
1485-1638 K: $ΔHf° = -415.100 + 15.544x10^{-3}T - 2.189x10^{-6}T^{2} + 894.900T^{-1}$
$ΔGf° = -415.100 - 15.544x10^{-3}TlnT + 2.189x10^{-6}T^{2} + 447.450T^{-1} + 195.178x10^{-3}T$
1638-1820 K: $ΔHf° = -490.032 + 18.716x10^{-3}T - 2.156x10^{-6}T^{2} - 200.900T^{-1}$
$ΔGf° = -490.032 - 18.716x10^{-3}TlnT + 2.156x10^{-6}T^{2} - 100.450T^{-1} + 264.658x10^{-3}T$
1820-1945 K: $ΔHf° = -467.609 + 20.956x10^{-3}T - 2.156x10^{-6}T^{2} - 200.900T^{-1}$
$ΔGf° = -467.609 - 20.956x10^{-3}TlnT + 2.156x10^{-6}T^{2} - 100.450T^{-1} + 269.152x10^{-3}T$
1945-2000 K: $ΔHf° = -460.477 + 12.983x10^{-3}T - 0.711x10^{-6}T^{2} - 969.000T^{-1}$
$ΔGf° = -460.477 - 12.983x10^{-3}TlnT + 0.711x10^{-6}T^{2} - 484.500T^{-1} + 208.020x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropies at 298 K from King (259). High-temperature data based on Christensen (93).

$Li_2Ti_3O_7(c)$
Lithium Trititanate
[Formation: $2Li(c,l) + 3Ti(c) + 3.5O_2(g) = Li_2Ti_3O_7(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	53.900	46.130	46.130	0	-844.000	-795.922	583.419
300	54.080	46.460	46.130	.100	-844.001	-795.619	579.601
400	61.400	63.110	48.360	5.900	-843.775	-779.518	425.904
453.7	64.085	71.030	50.556	9.289	-843.510	-770.905	371.345
453.7	64.085	71.030	50.556	9.289	-844.944	-770.905	371.345
500	66.400	77.370	52.750	12.310	-844.689	-763.357	333.659
600	70.480	89.850	57.933	19.150	-843.909	-747.171	272.153
700	74.130	100.990	63.290	26.390	-842.859	-731.102	228.257
800	77.560	111.120	68.658	33.970	-841.596	-715.239	195.392
900	80.850	120.440	73.896	41.890	-840.120	-699.522	169.865
1000	84.060	129.130	78.990	50.140	-838.419	-683.986	149.483

Phase change: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 54.953 + 29.990\times10^{-3}T - 8.881\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 54.953\times10^{-3}T + 14.995\times10^{-6}T^2 + 8.881\times10^{2}T^{-1} - 20.696$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -849.690 + 9.819\times10^{-3}T - 1.051\times10^{-6}T^2 + 851.500T^{-1}$

$\Delta Gf^\circ = -849.690 - 9.819\times10^{-3}T\ln T + 1.051\times10^{-6}T^2 + 425.750T^{-1} + 231.182\times10^{-3}T$

453.7-1000 K: $\Delta Hf^\circ = -848.811 - 0.377\times10^{-3}T + 9.877\times10^{-6}T^2 + 880.100T^{-1}$

$\Delta Gf^\circ = -848.811 + 0.377\times10^{-3}T\ln T - 9.877\times10^{-6}T^2 + 440.050T^{-1} + 171.759\times10^{-3}T$

Source: Data based on Kolotyrkin (279).

$LuFeO_3$(c)
Lutetium Ferrite
[Formation: Lu(c) + Fe(c) + 1.5O_2(g) = $LuFeO_3$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	27.340	27.600	27.600	0	-321.000	-301.737	221.177
300	27.340	27.770	27.603	.050	-320.993	-301.618	219.726
400	27.730	35.670	28.670	2.800	-320.575	-295.223	161.300
500	28.500	41.940	30.720	5.610	-320.187	-288.930	126.289
600	29.420	47.220	33.037	8.510	-319.805	-282.712	102.976
700	30.400	51.820	35.391	11.500	-319.431	-276.552	86.342
900	32.480	59.710	39.943	17.790	-318.745	-264.389	64.202
1000	33.540	63.190	42.100	21.090	-318.533	-258.368	56.466

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 22.450 + 10.940\times10^{-3}T + 1.450\times10^{5}T^{-2}$

$H°-H°_{298} = 22.450\times10^{-3}T + 5.470\times10^{-6}T^2 - 1.450\times10^{2}T^{-1} - 6.693$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -323.575 + 7.929\times10^{-3}T - 3.109\times10^{-6}T^2 + 145.200T^{-1}$

$\Delta Gf° = -323.575 - 7.929\times10^{-3}T\ln T + 3.109\times10^{-6}T^2 + 72.600T^{-1} + 116.675\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Vorob'ev (512). Other data based on Kaul (237).

LuO(g)
Lutetium Monoxide (ideal gas)
[Formation: Lu(c,l) + $0.5O_2(g)$ = LuO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.544	57.833	57.833	0	.500	-5.806	4.256
300	7.552	57.880	57.833	.014	.495	-5.845	4.258
400	7.943	60.108	58.136	.789	.275	-7.927	4.331
500	8.224	61.913	58.715	1.599	.075	-9.951	4.350
600	8.412	63.430	59.378	2.431	-.119	-11.939	4.349
700	8.541	64.737	60.053	3.279	-.314	-13.893	4.337
800	8.634	65.884	60.712	4.138	-.523	-15.815	4.320
900	8.703	66.905	61.344	5.005	-.753	-17.713	4.301
1000	8.755	67.824	61.946	5.878	-1.005	-19.584	4.280
1100	8.797	68.661	62.519	6.756	-1.284	-21.432	4.258
1200	8.830	69.428	63.064	7.637	-1.595	-23.248	4.234
1300	8.857	70.136	63.581	8.522	-1.943	-25.043	4.210
1400	8.880	70.793	64.072	9.409	-2.330	-26.797	4.183
1500	8.899	71.406	64.541	10.298	-2.760	-28.530	4.157
1600	8.916	71.981	64.989	11.188	-3.242	-30.236	4.130
1700	8.930	72.522	65.416	12.081	-3.773	-31.917	4.103
1800	8.942	73.033	65.825	12.974	-4.364	-33.546	4.073
1900	8.953	73.517	66.218	13.869	-5.014	-35.157	4.044
1936	8.956	73.685	66.355	14.191	-5.261	-35.733	4.034
1936	8.956	73.685	66.355	14.191	-9.718	-35.733	4.034
2000	8.962	73.976	66.593	14.765	-10.161	-36.567	3.996

Phase change: 1936 K, melting point of Lu; ΔH° = 4.457 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.437 + 0.350\times10^{-3}T - 0.886\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.437\times10^{-3}T + 0.175\times10^{-6}T^{2} + 0.886\times10^{2}T^{-1} - 2.828$

Formation equations (kcal/mol):

298.15-1936 K: $\Delta Hf^\circ = -0.269 + 0.925\times10^{-3}T - 1.831\times10^{-6}T^{2} + 195.500T^{-1}$

$\Delta Gf^\circ = -0.269 - 0.925\times10^{-3}T\ln T + 1.831\times10^{-6}T^{2} + 97.750T^{-1} - 14.947\times10^{-3}T$

1936-2000 K: $\Delta Hf^\circ = 3.390 - 6.628\times10^{-3}T - 0.076\times10^{-6}T^{2} + 66.000T^{-1}$

$\Delta Gf^\circ = 3.390 + 6.628\times10^{-3}T\ln T + 0.076\times10^{-6}T^{2} + 33.000T^{-1} - 70.588\times10^{-3}T$

Source: Data from Pedley (396).

$MgAl_2O_4(c)$
Magnesium Aluminate
[Formation: $Mg(c,l,g) + 2Al(c,l) + 2O_2(g) = MgAl_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^\circ_{298})/T$	$H°-H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	27.772	21.198	21.198	0	-549.500	-520.229	381.334
300	27.852	21.370	21.200	.051	-549.508	-520.047	378.849
400	32.980	30.173	22.363	3.124	-549.661	-510.194	278.754
500	35.810	37.861	24.713	6.574	-549.560	-500.337	218.695
600	37.736	44.568	27.475	10.256	-549.356	-490.504	178.664
700	39.234	50.502	30.349	14.107	-549.119	-480.714	150.084
800	40.505	55.825	33.206	18.095	-548.887	-470.963	128.659
900	41.644	60.663	35.993	22.203	-548.678	-461.231	112.001
922	41.876	61.672	36.594	23.122	-548.633	-459.098	108.823
922	41.876	61.672	36.594	23.122	-550.772	-459.098	108.823
933.61	41.999	62.196	36.909	23.609	-550.752	-457.944	107.199
933.61	41.999	62.196	36.909	23.609	-555.912	-457.944	107.199
1000	42.700	65.106	38.685	26.421	-555.731	-450.989	98.562
1100	43.703	69.223	41.276	30.742	-555.406	-440.532	87.524
1200	44.669	73.067	43.766	35.161	-555.031	-430.105	78.332
1300	45.609	76.680	46.161	39.675	-554.597	-419.701	70.557
1363	46.190	78.852	47.622	42.567	-554.299	-413.191	66.252
1363	46.190	78.852	47.622	42.567	-584.549	-413.191	66.252
1400	46.531	80.094	48.464	44.282	-584.220	-408.544	63.776
1500	47.439	83.335	50.682	48.980	-583.277	-396.032	57.701
1600	48.336	86.425	52.819	53.769	-582.257	-383.580	52.394
1700	49.226	89.383	54.885	58.647	-581.158	-371.198	47.720
1800	50.108	92.221	56.880	63.614	-579.981	-358.876	43.573
1900	50.986	94.954	58.812	68.669	-578.729	-346.625	39.870
2000	51.860	97.591	60.686	73.811	-577.400	-334.444	36.546

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 35.020 + 8.540\times10^{-3}T - 8.706\times10^{5}T^{-2}$
$H°-H^\circ_{298} = 35.020\times10^{-3}T + 4.270\times10^{-6}T^{2} + 8.706\times10^{2}T^{-1} - 13.741$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -553.945 + 6.233\times10^{-3}T - 1.578\times10^{-6}T^{2} + 813.100T^{-1}$
$\Delta Gf° = -553.945 - 6.233\times10^{-3}T\ln T + 1.578\times10^{-6}T^{2} + 406.550T^{-1} + 143.553\times10^{-3}T$
922-933.61 K: $\Delta Hf° = -555.269 + 5.367\times10^{-3}T - 1.264\times10^{-6}T^{2} + 551.400T^{-1}$
$\Delta Gf° = -555.269 - 5.367\times10^{-3}T\ln T + 1.264\times10^{-6}T^{2} + 275.700T^{-1} + 139.520\times10^{-3}T$
933.61-1363 K: $\Delta Hf° = -557.804 - 0.629\times10^{-3}T + 2.190\times10^{-6}T^{2} + 516.600T^{-1}$
$\Delta Gf° = -557.804 + 0.629\times10^{-3}T\ln T - 2.190\times10^{-6}T^{2} + 258.300T^{-1} + 104.473\times10^{-3}T$
1363-2000 K: $\Delta Hf° = -591.662 + 0.412\times10^{-3}T + 3.264\times10^{-6}T^{2} + 780.200T^{-1}$
$\Delta Gf° = -591.662 - 0.412\times10^{-3}T\ln T - 3.264\times10^{-6}T^{2} + 390.100T^{-1} + 138.220\times10^{-3}T$

Source: Data from JANAF (131).

$Mg_2Al_4Si_5O_{18}$(cordierite)
Magnesium Aluminum Silicate, Cordierite
[Formation: $2Mg(c,l,g) + 4Al(c,l) + 5Si(c,l) + 9O_2(g) = Mg_2Al_4Si_5O_{18}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	108.100	97.300	97.300	0	-2189.000	-2067.066	1515.181
300	108.500	97.970	97.303	.200	-2189.028	-2066.307	1505.285
400	127.530	131.750	101.775	11.990	-2189.775	-2025.263	1106.538
500	141.160	161.790	110.830	25.480	-2189.368	-1984.154	867.262
600	149.850	188.350	121.583	40.060	-2188.379	-1943.193	707.799
700	155.630	211.910	132.839	55.350	-2187.162	-1902.424	593.956
800	159.790	232.980	144.068	71.130	-2185.909	-1861.845	508.626
900	163.080	252.000	155.022	87.280	-2184.727	-1821.400	442.291
922	163.707	255.946	157.383	90.875	-2184.472	-1812.530	429.634
922	163.707	255.946	157.383	90.875	-2188.750	-1812.530	429.634
933.61	164.038	257.997	158.622	92.777	-2188.624	-1807.792	423.183
933.61	164.038	257.997	158.622	92.777	-2198.944	-1807.792	423.183
1000	165.930	269.330	165.600	103.730	-2198.094	-1779.978	389.009
1100	168.640	285.270	175.761	120.460	-2196.736	-1738.269	345.358
1200	171.390	300.060	185.510	137.460	-2195.284	-1696.655	308.999
1300	174.290	313.890	194.852	154.750	-2193.684	-1655.137	278.250
1363	176.268	322.183	200.550	165.787	-2192.620	-1629.086	261.212
1363	176.268	322.183	200.550	165.787	-2253.120	-1629.086	261.212
1400	177.430	326.920	203.827	172.330	-2252.169	-1612.160	251.666
1500	180.860	339.280	212.453	190.240	-2249.434	-1566.611	228.252
1600	184.620	351.070	220.751	208.510	-2246.427	-1521.193	207.783
1687	188.213	360.933	227.720	224.730	-2243.546	-1481.715	191.953
1687	188.213	360.933	227.720	224.730	-2303.956	-1481.715	191.953
1700	188.750	362.380	228.745	227.180	-2303.460	-1475.360	189.668

Phase changes: 922 K, melting point of Mg; $\Delta H° = 2.139$ kcal/mol.
933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.
1363 K, boiling point of Mg; $\Delta H° = 30.250$ kcal/mol.
1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1700 K: $Cp° = 141.686 + 27.836x10^{-3}T - 37.233x10^{5}T^{-2}$
$H°- H°_{298} = 141.686x10^{-3}T + 13.918x10^{-6}T^{2} + 37.233x10^{2}T^{-1} - 55.969$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -2204.344 + 19.567x10^{-3}T - 2.048x10^{-6}T^{2} + 2889.800T^{-1}$
$\Delta Gf° = -2204.344 - 19.567x10^{-3}T\ln T + 2.048x10^{-6}T^{2} + 1444.900T^{-1} + 555.054x10^{-3}T$
922-933.61 K: $\Delta Hf° = -2206.992 + 17.835x10^{-3}T - 1.420x10^{-6}T^{2} + 2366.400T^{-1}$
$\Delta Gf° = -2206.992 - 17.835x10^{-3}T\ln T + 1.420x10^{-6}T^{2} + 1183.200T^{-1} + 546.988x10^{-3}T$
933.61-1363 K: $\Delta Hf° = -2212.063 + 5.843x10^{-3}T + 5.488x10^{-6}T^{2} + 2296.800T^{-1}$
$\Delta Gf° = -2212.063 - 5.843x10^{-3}T\ln T - 5.488x10^{-6}T^{2} + 1148.400T^{-1} + 476.895x10^{-3}T$
1363-1687 K: $\Delta Hf° = -2279.778 + 7.925x10^{-3}T + 7.636x10^{-6}T^{2} + 2824.000T^{-1}$
$\Delta Gf° = -2279.778 - 7.925x10^{-3}T\ln T - 7.636x10^{-6}T^{2} + 1412.000T^{-1} + 544.389x10^{-3}T$
1687-1700 K: $\Delta Hf° = -2341.923 + 5.820x10^{-3}T + 9.391x10^{-6}T^{2} + 3316.500T^{-1}$
$\Delta Gf° = -2341.923 - 5.820x10^{-3}T\ln T - 9.391x10^{-6}T^{2} + 1658.250T^{-1} + 568.459x10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Charlu (75). Low-temperature heat capacities and entropy at 298 K from Weller (519). High-temperature data based on Pankratz (387).

MgB_2(c)
Magnesium Diboride
[Formation: Mg(c,l,g) + 2B(β) = MgB_2(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	11.430	8.600	8.600	0	-22.000	-21.395	15.683
300	11.440	8.671	8.601	.021	-22.000	-21.388	15.581
400*	13.000	12.190	9.070	1.248	-22.017	-21.189	11.577
500	13.960	15.198	10.002	2.598	-22.120	-20.969	9.165
600	14.670	17.808	11.091	4.030	-22.304	-20.725	7.549
700	15.300	20.117	12.218	5.529	-22.535	-20.440	6.382
800	15.900	22.199	13.338	7.089	-22.789	-20.124	5.498
900	16.530	24.108	14.429	8.711	-23.056	-19.769	4.801
922	16.664	24.509	14.665	9.076	-23.114	-19.692	4.668
922	16.664	24.509	14.665	9.076	-25.253	-19.692	4.668
1000	17.140	25.881	15.487	10.394	-25.466	-19.217	4.200
1100	17.705	27.541	16.507	12.137	-25.731	-18.593	3.694
1200	18.270	29.106	17.494	13.935	-26.001	-17.932	3.266
1300	18.833	30.591	18.445	15.790	-26.264	-17.230	2.897
1363	19.190	31.490	19.026	16.988	-26.429	-16.808	2.695
1363	19.190	31.490	19.026	16.988	-56.679	-16.808	2.695
1400	19.400	32.007	19.363	17.702	-56.632	-15.727	2.455

*Data above 300 K estimated.

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp^\circ = 12.021 + 5.310\text{x}10^{-3}T - 1.932\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 12.021\text{x}10^{-3}T + 2.655\text{x}10^{-6}T^{2} + 1.932\text{x}10^{2}T^{-1} - 4.468$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf^\circ = -20.380 - 2.568\text{x}10^{-3}T - 0.117\text{x}10^{-6}T^{2} - 251.700T^{-1}$
$\Delta Gf^\circ = -20.380 + 2.568\text{x}10^{-3}T\ln T + 0.117\text{x}10^{-6}T^{2} - 125.850T^{-1} - 16.655\text{x}10^{-3}T$
922-1363 K: $\Delta Hf^\circ = -21.703 - 3.434\text{x}10^{-3}T + 0.197\text{x}10^{-6}T^{2} - 513.400T^{-1}$
$\Delta Gf^\circ = -21.703 + 3.434\text{x}10^{-3}T\ln T - 0.197\text{x}10^{-6}T^{2} - 256.700T^{-1} - 20.688\text{x}10^{-3}T$
1363-1400 K: $\Delta Hf^\circ = -55.561 - 2.393\text{x}10^{-3}T + 1.271\text{x}10^{-6}T^{2} - 249.800T^{-1}$
$\Delta Gf^\circ = -55.561 + 2.393\text{x}10^{-3}T\ln T - 1.271\text{x}10^{-6}T^{2} - 124.900T^{-1} + 13.059\text{x}10^{-3}T$

Source: Data from JANAF (127) who estimated all above 300 K.

$MgB_4(c)$
Magnesium Tetraboride
[Formation: $Mg(c,l) + 4B(\beta) = MgB_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	16.810	12.410	12.410	0	-25.100	-24.790	18.171
300*	16.900	12.514	12.411	.031	-25.100	-24.783	18.054
400	19.000	17.671	13.098	1.829	-25.180	-24.680	13.485
500	20.800	22.106	14.466	3.820	-25.456	-24.519	10.717
600	22.500	26.053	16.075	5.987	-25.855	-24.303	8.852
700	23.890	29.626	17.759	8.307	-26.301	-24.002	7.494
800	25.270	32.907	19.450	10.766	-26.748	-23.642	6.459
900	26.540	35.959	21.118	13.357	-27.184	-23.223	5.639
922	26.786	36.603	21.480	13.944	-27.276	-23.129	5.482
922	26.786	36.603	21.480	13.944	-29.415	-23.129	5.482
1000	27.660	38.814	22.745	16.069	-29.741	-22.585	4.936
1100	28.610	41.496	24.330	18.883	-30.143	-21.878	4.347

*Data above 298 K estimated.

Phase change: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K:

$$Cp^\circ = 14.870 + 13.292\times10^{-3}T - 1.799\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 14.870\times10^{-3}T + 6.646\times10^{-6}T^{2} + 1.799\times10^{2}T^{-1} - 5.628$$

Formation equations (kcal/mol):

298.15-922 K:

$$\Delta Hf^\circ = -20.214 - 9.165\times10^{-3}T + 2.490\times10^{-6}T^{2} - 708.000T^{-1}$$

$$\Delta Gf^\circ = -20.214 + 9.165\times10^{-3}T\ln T - 2.490\times10^{-6}T^{2} - 354.000T^{-1} - 62.841\times10^{-3}T$$

922-1100 K:

$$\Delta Hf^\circ = -21.538 - 10.031\times10^{-3}T + 2.804\times10^{-6}T^{2} - 969.700T^{-1}$$

$$\Delta Gf^\circ = -21.538 + 10.031\times10^{-3}T\ln T - 2.804\times10^{-6}T^{2} - 484.850T^{-1} - 66.874\times10^{-3}T$$

Source: Data from JANAF (127) who estimated all above 298 K.

$MgC_2(c)$
Magnesium Dicarbide
[Formation: $Mg(c,l,g) + 2C(c) = MgC_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	13.440	13.000	13.000	0	20.000	19.271	-14.126
300	13.490	13.083	13.000	.025	20.006	19.267	-14.036
400	15.390	17.259	13.557	1.481	20.364	18.967	-10.363
500	16.350	20.807	14.661	3.073	20.683	18.577	-8.120
600	16.940	23.844	15.946	4.739	20.929	18.135	-6.606
700	17.360	26.489	17.268	6.455	21.103	17.654	-5.512
800	17.690	28.829	18.569	8.208	21.216	17.151	-4.685
900	17.960	30.928	19.827	9.991	21.274	16.643	-4.041
922	18.013	31.362	20.097	10.387	21.282	16.525	-3.917
922	18.013	31.362	20.097	10.387	19.143	16.525	-3.917
1000	18.200	32.833	21.034	11.799	19.151	16.298	-3.562
1100	18.410	34.578	22.187	13.630	19.134	16.032	-3.185
1200	18.610	36.189	23.287	15.482	19.080	15.728	-2.864
1300	18.810	37.686	24.338	17.353	19.001	15.465	-2.600
1363	18.923	38.579	24.976	18.542	18.937	15.274	-2.449
1363	18.923	38.579	24.976	18.542	-11.313	15.274	-2.449
1400	18.990	39.087	25.342	19.243	-11.211	15.994	-2.497
1500	19.170	40.403	26.302	21.151	-10.936	17.927	-2.612
1600	19.340	41.646	27.224	23.076	-10.656	19.843	-2.710
1700	19.510	42.823	28.107	25.018	-10.375	21.738	-2.795
1800	19.680	43.943	28.955	26.978	-10.085	23.622	-2.868
1900	19.840	45.011	29.772	28.954	-9.790	25.487	-2.932
2000	20.010	46.033	30.560	30.946	-9.491	27.337	-2.987

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 17.013 + 1.542\times10^{-3}T - 3.585\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.013\times10^{-3}T + 0.771\times10^{-6}T^{2} + 3.585\times10^{2}T^{-1} - 6.343$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf^\circ = 18.710 + 4.834\times10^{-3}T - 2.149\times10^{-6}T^{2} + 12.000T^{-1}$
$\Delta Gf^\circ = 18.710 - 4.834\times10^{-3}T\ln T + 2.149\times10^{-6}T^{2} + 6.000T^{-1} + 28.716\times10^{-3}T$
922-1363 K: $\Delta Hf^\circ = 17.386 + 3.968\times10^{-3}T - 1.835\times10^{-6}T^{2} - 249.700T^{-1}$
$\Delta Gf^\circ = 17.386 - 3.968\times10^{-3}T\ln T + 1.835\times10^{-6}T^{2} - 124.850T^{-1} + 24.683\times10^{-3}T$
1363-2000 K: $\Delta Hf^\circ = -16.472 + 5.009\times10^{-3}T - 0.761\times10^{-6}T^{2} + 13.900T^{-1}$
$\Delta Gf^\circ = -16.472 - 5.009\times10^{-3}T\ln T + 0.761\times10^{-6}T^{2} + 6.950T^{-1} + 58.430\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Other data from JANAF (127).

Mg_2C_3(c)
Dimagnesium Tricarbide
[Formation: $2Mg(c,l,g) + 3C(c) = Mg_2C_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	22.410	24.000	24.000	0	17.000	15.729	-11.529
300	22.500	24.139	24.000	.042	17.008	15.723	-11.454
400	25.660	31.105	24.930	2.470	17.484	15.222	-8.317
500	27.260	37.019	26.771	5.124	17.909	14.600	-6.382
600	28.250	42.084	28.912	7.903	18.225	13.916	-5.069
700	28.950	46.493	31.116	10.764	18.426	13.180	-4.115
800	29.490	50.395	33.286	13.687	18.528	12.418	-3.392
900	29.940	53.895	35.385	16.659	18.537	11.659	-2.831
922	30.028	54.619	35.835	17.319	18.531	11.483	-2.722
922	30.028	54.619	35.835	17.319	14.253	11.483	-2.722
1000	30.340	57.071	37.398	19.673	14.196	11.240	-2.456
1100	30.700	59.979	39.319	22.726	14.077	10.978	-2.181
1200	31.030	62.665	41.155	25.812	13.889	10.666	-1.942
1300	31.350	65.161	42.906	28.931	13.658	10.431	-1.754
1363	31.539	66.649	43.969	30.912	13.486	10.239	-1.642
1363	31.539	66.649	43.969	30.912	-47.014	10.239	-1.642
1400	31.650	67.495	44.580	32.081	-46.837	11.789	-1.840
1500	31.950	69.689	46.182	35.261	-46.355	15.958	-2.325
1600	32.240	71.760	47.716	38.471	-45.861	20.101	-2.746
1700	32.520	73.723	49.188	41.709	-45.363	24.203	-3.111
1800	32.800	75.590	50.604	44.975	-44.850	28.284	-3.434
1900	33.070	77.371	51.966	48.269	-44.326	32.333	-3.719
2000	33.350	79.074	53.279	51.590	-43.793	36.357	-3.973

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 28.373 + 2.562\times10^{-3}T - 5.980\times10^{5}T^{-2}$
$H°-H°_{298} = 28.373\times10^{-3}T + 1.281\times10^{-6}T^{2} + 5.980\times10^{2}T^{-1} - 10.579$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = 14.832 + 7.533\times10^{-3}T - 3.793\times10^{-6}T^{2} + 77.300T^{-1}$
$\Delta Gf° = 14.832 - 7.533\times10^{-3}T\ln T + 3.793\times10^{-6}T^{2} + 38.650T^{-1} + 44.362\times10^{-3}T$
922-1363 K: $\Delta Hf° = 12.185 + 5.801\times10^{-3}T - 3.165\times10^{-6}T^{2} - 446.100T^{-1}$
$\Delta Gf° = 12.185 - 5.801\times10^{-3}T\ln T + 3.165\times10^{-6}T^{2} - 223.050T^{-1} + 36.297\times10^{-3}T$
1363-2000 K: $\Delta Hf° = -55.530 + 7.883\times10^{-3}T - 1.017\times10^{-6}T^{2} + 81.100T^{-1}$
$\Delta Gf° = -55.530 - 7.883\times10^{-3}T\ln T + 1.017\times10^{-6}T^{2} + 40.550T^{-1} + 103.790\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Other data from JANAF (127).

$MgCO_3(c)$
Magnesium Carbonate
[Formation: $Mg(c,l) + C(c) + 1.5O_2(g) = MgCO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	18.190	15.560	15.560	0	-266.035	-246.020	180.335
300	18.250	15.670	15.560	.034	-266.035	-245.894	179.131
400	21.650	21.430	16.315	2.046	-265.943	-239.187	130.684
500	23.880	26.520	17.866	4.327	-265.714	-232.530	101.637
600	25.660	31.030	19.687	6.806	-265.410	-225.913	82.288
700	27.240	35.110	21.606	9.453	-265.048	-219.359	68.486
800	28.700	38.840	23.528	12.250	-264.630	-212.862	58.151
900	29.910	42.300	25.423	15.189	-264.150	-206.415	50.124
922	30.247	43.026	25.835	15.851	-264.037	-205.009	48.594
922	30.247	43.026	25.835	15.851	-266.176	-205.009	48.594
1000	31.440	45.540	27.274	18.266	-265.737	-199.857	43.678

Phase change: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 19.352 + 12.526x10^{-3}T - 4.343x10^{5}T^{-2}$

$H°- H°_{298} = 19.352x10^{-3}T + 6.263x10^{-6}T^{2} + 4.343x10^{2}T^{-1} - 7.783$

Formation equations (kcal/mol):

298.15-922 K: $ΔHf° = -266.932 - 0.154x10^{-3}T + 3.355x10^{-6}T^{2} + 192.300T^{-1}$

$ΔGf° = -266.932 + 0.154x10^{-3}T\ln T - 3.355x10^{-6}T^{2} + 96.150T^{-1} + 69.180x10^{-3}T$

922-1000 K: $ΔHf° = -268.256 - 1.020x10^{-3}T + 3.669x10^{-6}T^{2} - 69.400T^{-1}$

$ΔGf° = -268.256 + 1.020x10^{-3}T\ln T - 3.669x10^{-6}T^{2} - 34.700T^{-1} + 65.147x10^{-3}T$

Source: Data from Chang (74).

$MgCr_2O_4(c)$
Magnesium Chromate
[Formation: $Mg(c,l,g) + 2Cr(c) + 2O_2(g) = MgCr_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	30.363	25.340	25.340	0	-426.300	-398.936	292.424
300	30.497	25.528	25.341	.056	-426.301	-398.767	290.498
311.5	31.060	26.686	25.370	.410	-426.312	-397.711	279.032
400	35.390	35.062	26.607	3.382	-426.167	-389.600	212.865
500	37.920	43.256	29.138	7.059	-425.835	-380.492	166.311
600	39.502	50.319	32.094	10.935	-425.451	-371.454	135.300
700	40.621	56.497	35.148	14.944	-425.066	-362.482	113.171
800	41.481	61.979	38.165	19.051	-424.701	-353.572	96.590
900	42.177	66.907	41.090	23.235	-424.356	-344.696	83.703
922	42.306	67.927	41.719	24.164	-424.284	-342.754	81.245
922	42.306	67.927	41.719	24.164	-426.423	-342.754	81.245
1000	42.762	71.381	43.898	27.483	-426.183	-335.694	73.365
1100	43.263	75.481	46.586	31.784	-425.932	-326.658	64.900
1200	43.698	79.265	49.154	36.133	-425.757	-317.636	57.849
1300	44.079	82.778	51.607	40.522	-425.672	-308.636	51.886
1363	44.289	84.869	53.097	43.306	-425.663	-302.994	48.583
1363	44.289	84.869	53.097	43.306	-455.913	-302.994	48.583
1400	44.412	86.057	53.952	44.947	-455.777	-298.845	46.651
1500	44.702	89.131	56.196	49.403	-455.450	-287.627	41.907
1600	44.953	92.024	58.345	53.886	-455.202	-276.447	37.760
1700	45.168	94.756	60.407	58.393	-455.024	-265.302	34.106
1800	45.347	97.343	62.388	62.919	-454.918	-254.121	30.854

<u>Phase change</u>: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

<u>Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations</u>:

298.15-1800 K: $Cp° = 40.245 + 3.318\times10^{-3}T - 9.664\times10^{5}T^{-2}$
$H°-H°_{298} = 40.245\times10^{-3}T + 1.659\times10^{-6}T^{2} + 9.664\times10^{2}T^{-1} - 15.388$

<u>Formation equations (kcal/mol)</u>:

298.15-311.5 K: $\Delta Hf° = -434.494 + 26.258\times10^{-3}T - 28.869\times10^{-6}T^{2} + 874.100T^{-1}$
$\Delta Gf° = -434.494 - 26.258\times10^{-3}T\ln T + 28.869\times10^{-6}T^{2} + 437.050T^{-1} + 255.347\times10^{-3}T$
311.5-922 K: $\Delta Hf° = -432.499 + 11.924\times10^{-3}T - 4.317\times10^{-6}T^{2} + 901.300T^{-1}$
$\Delta Gf° = -432.499 - 11.924\times10^{-3}T\ln T + 4.317\times10^{-6}T^{2} + 450.650T^{-1} + 174.152\times10^{-3}T$
922-1363 K: $\Delta Hf° = -433.823 + 11.058\times10^{-3}T - 4.003\times10^{-6}T^{2} + 639.600T^{-1}$
$\Delta Gf° = -433.823 - 11.058\times10^{-3}T\ln T + 4.003\times10^{-6}T^{2} + 319.800T^{-1} + 170.120\times10^{-3}T$
1363-1800 K: $\Delta Hf° = -467.680 + 12.099\times10^{-3}T - 2.929\times10^{-6}T^{2} + 903.200T^{-1}$
$\Delta Gf° = -467.680 - 12.099\times10^{-3}T\ln T + 2.929\times10^{-6}T^{2} + 451.600T^{-1} + 203.866\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (<u>391</u>). Low-temperature heat capacities and entropy at 298 K from Shomate (<u>449</u>). High-temperature data based on Naylor (<u>350</u>) and Landa (<u>291</u>).

$MgFe_2O_4(c)$
Magnesium Ferrite
[Formation: $Mg(c,l,g) + 2Fe(c) + 2O_2(g) = MgFe_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	34.350	29.600	29.600	0	-341.400	-314.787	230.742
300	34.474	29.813	29.600	.064	-341.395	-314.620	229.198
400	39.304	40.456	31.019	3.775	-340.966	-305.753	167.054
500	42.451	49.568	33.840	7.864	-340.342	-297.022	129.827
600	47.244	57.678	37.145	12.320	-339.536	-288.423	105.057
670	53.615	63.205	39.578	15.830	-338.693	-282.503	92.149
670	45.536	63.205	39.578	15.830	-338.693	-282.503	92.149
700	45.536	65.200	40.634	17.196	-338.500	-279.991	87.416
800	45.536	71.280	44.092	21.750	-337.994	-271.676	74.217
900	45.536	76.644	47.418	26.303	-337.744	-263.399	63.961
922	45.536	77.744	48.129	27.305	-337.737	-261.585	62.005
922	45.536	77.744	48.129	27.305	-339.876	-261.585	62.005
1000	45.536	81.441	50.584	30.857	-340.033	-254.964	55.722
1043	45.536	83.358	51.896	32.815	-340.403	-251.300	52.657
1100	45.536	85.781	53.590	35.410	-340.622	-246.423	48.959
1185	45.536	89.171	56.023	39.281	-340.664	-239.146	44.105
1185	45.536	89.171	56.023	39.281	-341.094	-239.146	44.105
1200	45.536	89.744	56.441	39.964	-341.036	-237.858	43.319
1230	45.536	90.868	57.266	41.330	-340.924	-235.279	41.805
1230	42.111	91.112	57.266	41.630	-340.624	-235.279	41.805
1300	43.110	93.470	59.152	44.613	-340.589	-229.270	38.543
1363	44.010	95.531	60.787	47.357	-340.537	-223.898	35.900
1363	44.010	95.531	60.787	47.357	-370.787	-223.898	35.900
1400	44.538	96.717	61.721	48.995	-370.601	-219.913	34.330
1500	45.965	99.839	64.159	53.520	-370.035	-209.172	30.476
1600	47.393	102.851	66.483	58.188	-369.380	-198.466	27.109
1667	48.349	104.815	67.985	61.396	-368.890	-191.320	25.082
1667	48.349	104.815	67.985	61.396	-369.290	-191.320	25.082
1700	48.820	105.767	68.709	62.999	-369.084	-187.799	24.143
1800	50.248	108.598	70.847	67.952	-368.403	-177.151	21.509

Phase changes:
670 K, second order transition point of $MgFe_2O_4$; ΔH° = 0.kcal/mol.
922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0.kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1230 K, α - β transition point of $MgFe_2O_4$; ΔH° = 0.300 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-670 K: $Cp° = 23.881 + 39.930\times10^{-3}T - 1.276\times10^{5}T^{-2}$
$H°-H°_{298} = 23.881\times10^{-3}T + 19.965\times10^{-6}T^{2} + 1.276\times10^{2}T^{-1} - 9.323$
670-1230 K: $Cp° = 45.536$
$H°-H°_{298} = 45.536\times10^{-3}T - 14.679$
1230-1800 K: $Cp° = 24.554 + 14.274\times10^{-3}T$
$H°-H°_{298} = 24.554\times10^{-3}T + 7.137\times10^{-6}T^{2} + 0.631$

Formation equations (kcal/mol):

298.15-670 K: $\Delta Hf° = -344.941 + 4.720\times10^{-3}T + 5.429\times10^{-6}T^{2} + 492.300T^{-1}$
$\Delta Gf° = -344.941 - 4.720\times10^{-3}T\ln T - 5.429\times10^{-6}T^{2} + 246.150T^{-1} + 126.879\times10^{-3}T$
670-922 K: $\Delta Hf° = -350.297 + 26.375\times10^{-3}T - 14.536\times10^{-6}T^{2} + 364.700T^{-1}$
$\Delta Gf° = -350.297 - 26.375\times10^{-3}T\ln T + 14.536\times10^{-6}T^{2} + 182.350T^{-1} + 262.554\times10^{-3}T$
922-1043 K: $\Delta Hf° = -351.621 + 25.509\times10^{-3}T - 14.222\times10^{-6}T^{2} + 103.000T^{-1}$
$\Delta Gf° = -351.621 - 25.509\times10^{-3}T\ln T + 14.222\times10^{-6}T^{2} + 51.500T^{-1} + 258.521\times10^{-3}T$
1043-1185 K: $\Delta Hf° = -304.499 - 62.453\times10^{-3}T + 27.200\times10^{-6}T^{2} - 354.000T^{-1}$
$\Delta Gf° = -304.499 + 62.453\times10^{-3}T\ln T - 27.200\times10^{-6}T^{2} - 177.000T^{-1} - 354.568\times10^{-3}T$
1185-1230 K: $\Delta Hf° = -351.727 + 14.057\times10^{-3}T - 4.182\times10^{-6}T^{2} - 116.000T^{-1}$
$\Delta Gf° = -351.727 - 14.057\times10^{-3}T\ln T + 4.182\times10^{-6}T^{2} - 58.000T^{-1} + 139.514\times10^{-3}T$
1230-1363 K: $\Delta Hf° = -336.417 - 6.925\times10^{-3}T + 2.955\times10^{-6}T^{2} - 116.000T^{-1}$
$\Delta Gf° = -336.417 + 6.925\times10^{-3}T\ln T - 2.955\times10^{-6}T^{2} - 58.000T^{-1} + 36.563\times10^{-3}T$
1363-1667 K: $\Delta Hf° = -370.274 - 5.884\times10^{-3}T + 4.029\times10^{-6}T^{2} + 147.600T^{-1}$
$\Delta Gf° = -370.274 + 5.884\times10^{-3}T\ln T - 4.029\times10^{-6}T^{2} + 73.800T^{-1} + 70.309\times10^{-3}T$
1667-1800 K: $\Delta Hf° = -536.064 + 91.110\times10^{-3}T - 15.233\times10^{-6}T^{2} + 95546.000T^{-1}$
$\Delta Gf° = -536.064 - 91.110\times10^{-3}T\ln T + 15.233\times10^{-6}T^{2} + 47773.000T^{-1} + 840.066\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Parker (391). Low-temperature heat capacities from King (258). High-temperature data based on Bonnickson (51).

MgH(g)
Magnesium Hydride (ideal gas)
[Formation: $Mg(c,l,g) + 0.5H_2(g) = MgH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.070	46.150	46.150	0	40.400	33.621	-24.645
300	7.074	46.194	46.151	.013	40.396	33.580	-24.463
400	7.298	48.257	46.430	.731	40.157	31.343	-17.125
500	7.572	49.915	46.967	1.474	39.911	29.165	-12.748
600	7.834	51.319	47.577	2.245	39.666	27.043	-9.850
700	8.060	52.544	48.201	3.040	39.416	24.960	-7.793
800	8.248	53.633	48.813	3.856	39.157	22.909	-6.258
900	8.403	54.614	49.405	4.688	38.882	20.899	-5.075
922	8.431	54.817	49.532	4.873	38.821	20.456	-4.849
922	8.431	54.817	49.532	4.873	36.682	20.456	-4.849
1000	8.531	55.506	49.971	5.535	36.454	19.088	-4.172
1100	8.638	56.324	50.511	6.394	36.150	17.364	-3.450
1200	8.728	57.080	51.028	7.262	35.820	15.667	-2.853
1300	8.806	57.781	51.520	8.139	35.474	14.016	-2.356
1363	8.848	58.199	51.819	8.695	35.242	12.962	-2.078
1363	8.848	58.199	51.819	8.695	4.992	12.962	-2.078
1400	8.873	58.436	51.991	9.023	4.996	13.177	-2.057
1500	8.933	59.051	52.442	9.914	5.006	13.759	-2.005
1600	8.986	59.629	52.873	10.810	5.017	14.343	-1.959
1700	9.034	60.175	53.286	11.711	5.027	14.926	-1.919
1800	9.078	60.693	53.684	12.616	5.038	15.507	-1.883
1900	9.119	61.185	54.066	13.526	5.048	16.089	-1.851
2000	9.157	61.654	54.434	14.440	5.057	16.670	-1.822

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.283 + 1.152\times10^{-3}T - 0.495\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.283\times10^{-3}T + 0.576\times10^{-6}T^{2} + 0.495\times10^{2}T^{-1} - 2.389$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf^\circ = 40.628 - 1.088\times10^{-3}T - 1.021\times10^{-6}T^{2} + 55.850T^{-1}$

$\Delta Gf^\circ = 40.628 + 1.088\times10^{-3}T\ln T + 1.021\times10^{-6}T^{2} + 27.925T^{-1} - 30.318\times10^{-3}T$

922-1363 K: $\Delta Hf^\circ = 39.304 - 1.954\times10^{-3}T - 0.708\times10^{-6}T^{2} - 205.850T^{-1}$

$\Delta Gf^\circ = 39.304 + 1.954\times10^{-3}T\ln T + 0.708\times10^{-6}T^{2} - 102.925T^{-1} - 34.351\times10^{-3}T$

1363-2000 K: $\Delta Hf^\circ = 5.447 - 0.913\times10^{-3}T + 0.367\times10^{-6}T^{2} + 57.750T^{-1}$

$\Delta Gf^\circ = 5.447 + 0.913\times10^{-3}T\ln T - 0.367\times10^{-6}T^{2} + 28.875T^{-1} - 0.604\times10^{-3}T$

Source: Data from JANAF (127).

MgH_2(c,l)
Magnesium Dihydride
[Formation: Mg(c) + H_2(g) = MgH_2(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.449	7.433	7.433	0	-18.100	-8.683	6.365
300	8.465	7.485	7.433	.016	-18.108	-8.624	6.282
400	9.308	10.036	7.776	.904	-18.524	-5.400	2.950
500	10.151	12.204	8.450	1.877	-18.889	-2.078	.908
600	10.994	14.129	9.237	2.935	-19.197	1.319	-.480
600	17.925	19.706	9.237	6.281	-15.851	1.319	-.480
700	17.925	22.469	10.936	8.073	-15.455	4.149	-1.295
800	17.925	24.863	12.531	9.866	-15.090	6.921	-1.891
900	17.925	26.974	14.021	11.658	-14.760	9.657	-2.345

Phase change: 600 K, melting point of MgH_2; ΔH° = 3.346 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 5.866 + 8.552\times10^{-3}T + 0.029\times10^{5}T^{-2}$
$H°-H°_{298} = 5.866\times10^{-3}T + 4.276\times10^{-6}T^{2} - 0.029\times10^{2}T^{-1} - 2.119$
600-900 K: $Cp° = 17.925$
$H°-H°_{298} = 17.925\times10^{-3}T - 4.474$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = -16.649 - 5.733\times10^{-3}T + 2.469\times10^{-6}T^{2} + 11.700T^{-1}$
$\Delta Gf° = -16.649 + 5.733\times10^{-3}T\ln T - 2.469\times10^{-6}T^{2} + 5.850T^{-1} - 5.275\times10^{-3}T$
600-900 K: $\Delta Hf° = -19.004 + 6.326\times10^{-3}T - 1.807\times10^{-6}T^{2} + 14.600T^{-1}$
$\Delta Gf° = -19.004 - 6.326\times10^{-3}T\ln T + 1.807\times10^{-6}T^{2} + 7.300T^{-1} + 73.220\times10^{-3}T$

Source: Data from Gurvich (196).

$MgMoO_4(c)$
Magnesium Molybdate
[Formation: $Mg(c,l) + Mo(c) + 2O_2(g) = MgMoO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	26.570	28.400	28.400	0	-334.800	-309.675	226.995
300*	26.640	28.560	28.400	.049	-334.799	-309.517	225.480
400	29.800	36.690	29.485	2.882	-334.583	-301.118	164.521
500	32.030	43.590	31.632	5.979	-334.194	-292.794	127.979
600	33.740	49.590	34.137	9.272	-333.702	-284.556	103.648
700	35.080	54.900	36.736	12.715	-333.146	-276.410	86.298
800	36.150	59.650	39.303	16.278	-332.550	-268.346	73.308
900	37.000	63.960	41.807	19.938	-331.928	-260.352	63.221
922	37.143	64.855	42.346	20.754	-331.789	-258.608	61.299
922	37.143	64.855	42.346	20.754	-333.928	-258.608	61.299
1000	37.650	67.900	44.228	23.672	-333.435	-252.269	55.133
1100	38.130	71.510	46.545	27.462	-332.807	-244.182	48.514
1200	38.440	74.840	48.763	31.292	-332.201	-236.151	43.008

*Data above 298 K estimated.

Phase change: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 29.896 + 8.498\text{x}10^{-3}T - 5.209\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 29.896\text{x}10^{-3}T + 4.249\text{x}10^{-6}T^{2} + 5.209\text{x}10^{2}T^{-1} - 11.038$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf^\circ = -338.259 + 5.916\text{x}10^{-3}T + 0.670\text{x}10^{-6}T^{2} + 487.800T^{-1}$

$\Delta Gf^\circ = -338.259 - 5.916\text{x}10^{-3}T\ln T - 0.670\text{x}10^{-6}T^{2} + 243.900T^{-1} + 127.036\text{x}10^{-3}T$

922-1200 K: $\Delta Hf^\circ = -339.583 + 5.050\text{x}10^{-3}T + 0.984\text{x}10^{-6}T^{2} + 226.100T^{-1}$

$\Delta Gf^\circ = -339.583 - 5.050\text{x}10^{-3}T\ln T - 0.984\text{x}10^{-6}T^{2} + 113.050T^{-1} + 123.003\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Barany (18). Low-temperature heat capacities and entropy at 298 K from Weller (522). Data above 298 K estimated.

MgN(g)
Magnesium Nitride (ideal gas)
[Formation: $Mg(c,l,g) + 0.5N_2(g) = MgN(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.823	53.713	53.713	0	69.000	62.137	-45.547
300	7.832	53.761	53.714	.014	68.996	62.095	-45.236
400	8.208	56.070	54.025	.818	68.842	59.818	-32.682
500	8.449	57.929	54.625	1.652	68.686	57.578	-25.167
600	8.607	59.484	55.309	2.505	68.516	55.375	-20.170
700	8.716	60.820	56.004	3.371	68.325	53.200	-16.609
800	8.794	61.989	56.680	4.247	68.107	51.051	-13.946
900	8.854	63.028	57.328	5.130	67.859	48.940	-11.884
922	8.864	63.242	57.467	5.325	67.802	48.474	-11.490
922	8.864	63.242	57.467	5.325	65.663	48.474	-11.490
1000	8.901	63.964	57.947	6.017	65.442	47.022	-10.277
1100	8.939	64.814	58.533	6.909	65.140	45.192	-8.979
1200	8.971	65.593	59.089	7.805	64.806	43.391	-7.903
1300	8.999	66.312	59.617	8.703	64.449	41.634	-6.999
1363	9.014	66.738	59.936	9.271	64.209	40.515	-6.496
1363	9.014	66.738	59.936	9.271	33.959	40.515	-6.496
1400	9.023	66.980	60.119	9.605	33.956	40.692	-6.352
1500	9.046	67.603	60.598	10.508	33.948	41.172	-5.999
1600	9.066	68.188	61.054	11.414	33.939	41.654	-5.690
1700	9.085	68.738	61.490	12.321	33.927	42.135	-5.417
1800	9.103	69.258	61.908	13.230	33.916	42.619	-5.175
1900	9.119	69.750	62.307	14.142	33.904	43.105	-4.958
2000	9.136	70.219	62.692	15.054	33.890	43.588	-4.763

*Data estimated.

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.697 + 0.252\times10^{-3}T - 0.844\times10^{5}T^{-2}$

$H° - H°_{298} = 8.697\times10^{-3}T + 0.126\times10^{-6}T^{2} + 0.844\times10^{2}T^{-1} - 2.887$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = 68.760 + 0.295\times10^{-3}T - 1.557\times10^{-6}T^{2} + 86.450T^{-1}$

$\Delta Gf° = 68.760 - 0.295\times10^{-3}T\ln T + 1.557\times10^{-6}T^{2} + 43.225T^{-1} - 21.481\times10^{-3}T$

922-1363 K: $\Delta Hf° = 67.437 - 0.571\times10^{-3}T - 1.243\times10^{-6}T^{2} - 175.250T^{-1}$

$\Delta Gf° = 67.437 + 0.571\times10^{-3}T\ln T + 1.243\times10^{-6}T^{2} - 87.625T^{-1} - 25.513\times10^{-3}T$

1363-2000 K: $\Delta Hf° = 33.579 + 0.470\times10^{-3}T - 0.169\times10^{-6}T^{2} + 88.350T^{-1}$

$\Delta Gf° = 33.579 - 0.470\times10^{-3}T\ln T + 0.169\times10^{-6}T^{2} + 44.175T^{-1} + 8.233\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$Mg_3N_2(c)$
Trimagnesium Dinitride
[Formation: $3Mg(c,l,g) + N_2(g) = Mg_3N_2(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	24.980	21.000	21.000	0	-110.100	-95.729	70.170
300	25.000	21.150	21.000	.046	-110.100	-95.636	69.670
400	25.730	28.440	21.985	2.582	-110.091	-90.820	49.621
500	26.460	34.260	23.876	5.192	-110.101	-86.008	37.594
600	27.190	39.150	26.027	7.874	-110.130	-81.177	29.568
700	27.920	43.400	28.214	10.630	-110.183	-76.348	23.837
800	28.650	47.170	30.347	13.458	-110.264	-71.514	19.536
823	28.820	47.980	30.826	14.119	-110.286	-70.397	18.694
823	29.600	48.250	30.826	14.339	-110.066	-70.397	18.694
900	29.600	50.900	32.436	16.618	-110.116	-66.671	16.190
922	29.600	51.615	32.885	17.269	-110.138	-65.621	15.555
922	29.600	51.615	32.885	17.269	-116.555	-65.621	15.555
1000	29.600	54.020	34.442	19.578	-116.682	-61.324	13.402
1061	29.600	55.770	35.618	21.384	-116.809	-57.951	11.937
1061	29.540	56.020	35.618	21.644	-116.549	-57.951	11.937
1100	29.540	57.080	36.356	22.796	-116.652	-55.790	11.084
1200	29.540	59.650	38.192	25.750	-116.988	-50.250	9.152
1300	29.540	62.020	39.940	28.704	-117.395	-44.640	7.505
1363	29.540	63.419	40.994	30.565	-117.700	-41.169	6.601
1363	29.540	63.419	40.994	30.565	-208.450	-41.169	6.601
1400	29.540	64.210	41.597	31.658	-208.214	-36.633	5.719
1500	29.540	66.250	43.175	34.612	-207.580	-24.406	3.556
1600	29.540	68.150	44.671	37.566	-206.953	-12.204	1.667
1700	29.540	69.940	46.105	40.520	-206.333	-.052	.007
1800	29.540	71.630	47.478	43.474	-205.715	12.065	-1.465
1900	29.540	73.230	48.794	46.428	-205.105	24.143	-2.777
2000	29.540	74.740	50.049	49.382	-204.500	36.204	-3.956

Phase changes:
823 K, α - β transition point of Mg_3N_2; ΔH° = 0.220 kcal/mol.
922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1061 K, β - γ transition point of Mg_3N_2; ΔH° = 0.260 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-823 K: $Cp° = 22.833 + 7.270\times10^{-3}T - 0.018\times10^{5}T^{-2}$
$H°-H°_{298} = 22.833\times10^{-3}T + 3.635\times10^{-6}T^{2} + 0.018\times10^{2}T^{-1} - 7.137$
823-1061 K: $Cp° = 29.600$
$H°-H°_{298} = 29.600\times10^{-3}T - 10.022$
1061-2000 K: $Cp° = 29.540$
$H°-H°_{298} = 29.540\times10^{-3}T - 9.698$

Formation equations (kcal/mol):

298.15-823 K: $\Delta Hf° = -110.278 + 0.887\times10^{-3}T - 1.118\times10^{-6}T^{2} + 4.000T^{-1}$
$\Delta Gf° = -110.278 - 0.887\times10^{-3}T\ln T + 1.118\times10^{-6}T^{2} + 2.000T^{-1} + 53.497\times10^{-3}T$
823-922 K: $\Delta Hf° = -113.163 + 7.654\times10^{-3}T - 4.753\times10^{-6}T^{2} + 2.200T^{-1}$
$\Delta Gf° = -113.163 - 7.654\times10^{-3}T\ln T + 4.753\times10^{-6}T^{2} + 1.100T^{-1} + 99.438\times10^{-3}T$
922-1061 K: $\Delta Hf° = -117.134 + 5.056\times10^{-3}T - 3.811\times10^{-6}T^{2} - 782.900T^{-1}$
$\Delta Gf° = -117.134 - 5.056\times10^{-3}T\ln T + 3.811\times10^{-6}T^{2} - 391.450T^{-1} + 87.340\times10^{-3}T$
1061-1363 K: $\Delta Hf° = -116.811 + 4.996\times10^{-3}T - 3.811\times10^{-6}T^{2} - 782.900T^{-1}$
$\Delta Gf° = -116.811 - 4.996\times10^{-3}T\ln T + 3.811\times10^{-6}T^{2} - 391.450T^{-1} + 86.617\times10^{-3}T$
1363-2000 K: $\Delta Hf° = -218.383 + 8.119\times10^{-3}T - 0.589\times10^{-6}T^{2} + 7.900T^{-1}$
$\Delta Gf° = -218.383 - 8.119\times10^{-3}T\ln T + 0.589\times10^{-6}T^{2} + 3.950T^{-1} + 187.857\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Other data from Douglas (126).

$Mg(NO_3)_2(c)$
Magnesium Nitrate
[Formation: $Mg(c) + N_2(g) + 3O_2(g) = Mg(NO_3)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	33.920	39.150	39.150	0	-188.970	-140.835	103.234
300	34.040	39.360	39.150	.063	-188.970	-140.535	102.378
400	40.376	50.004	40.559	3.778	-188.692	-124.418	67.978
500	46.800	59.704	43.430	8.137	-187.868	-108.436	47.397
600	53.216	68.804	46.907	13.138	-186.511	-92.664	33.752

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp^\circ = 14.808 + 64.052\times10^{-3}T - 0.086\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.808\times10^{-3}T + 32.026\times10^{-6}T^{2} + 0.086\times10^{2}T^{-1} - 7.291$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf^\circ = -185.573 - 18.542\times10^{-3}T + 28.540\times10^{-6}T^{2} - 121.000T^{-1}$

$\Delta Gf^\circ = -185.573 + 18.542\times10^{-3}T\ln T - 28.540\times10^{-6}T^{2} - 60.500T^{-1} + 53.596\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Shomate (450). High-temperature data based on Shomate (454).

MgOH(g)
Magnesium Monohydroxide (ideal gas)
[Formation: $Mg(c,l,g) + 0.5O_2(g) + 0.5H_2(g) = MgOH(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.360	52.916	52.916	0	-52.000	-53.491	39.209
300	8.382	52.968	52.918	.015	-52.009	-53.500	38.974
400	9.485	55.535	53.260	.910	-52.426	-53.933	29.467
500	10.342	57.748	53.940	1.904	-52.786	-54.268	23.720
600	10.970	59.692	54.740	2.971	-53.112	-54.530	19.862
700	11.443	61.421	55.574	4.093	-53.425	-54.741	17.091
800	11.817	62.974	56.403	5.257	-53.735	-54.911	15.001
900	12.128	64.384	57.213	6.454	-54.051	-55.034	13.364
922	12.187	64.678	57.388	6.721	-54.121	-55.062	13.052
922	12.187	64.678	57.388	6.721	-56.260	-55.062	13.052
1000	12.394	65.676	57.995	7.681	-56.514	-54.955	12.010
1100	12.628	66.869	58.749	8.932	-56.845	-54.786	10.885
1200	12.835	67.976	59.472	10.205	-57.194	-54.585	9.941
1300	13.019	69.011	60.166	11.498	-57.552	-54.340	9.135
1363	13.122	69.630	60.589	12.322	-57.787	-54.199	8.690
1363	13.122	69.630	60.589	12.322	-88.037	-54.199	8.690
1400	13.183	69.982	60.833	12.809	-88.035	-53.281	8.317
1500	13.330	70.897	61.474	14.134	-88.026	-50.802	7.402
1600	13.462	71.761	62.090	15.474	-88.010	-48.319	6.600
1700	13.579	72.581	62.683	16.826	-87.989	-45.839	5.893
1800	13.685	73.360	63.254	18.190	-87.964	-43.359	5.264
1900	13.779	74.103	63.807	19.563	-87.938	-40.882	4.702
2000	13.864	74.812	64.340	20.945	-87.910	-38.406	4.197

*Data estimated.

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.295 + 2.138\times10^{-3}T - 2.287\times10^{5}T^{-2}$
$H°-H°_{298} = 10.295\times10^{-3}T + 1.069\times10^{-6}T^{2} + 2.287\times10^{2}T^{-1} - 3.932$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -52.139 - 1.691\times10^{-3}T - 0.780\times10^{-6}T^{2} + 212.450T^{-1}$
$\Delta Gf° = -52.139 + 1.691\times10^{-3}T\ln T + 0.780\times10^{-6}T^{2} + 106.225T^{-1} - 15.596\times10^{-3}T$
922-1363 K: $\Delta Hf° = -53.463 - 2.557\times10^{-3}T - 0.466\times10^{-6}T^{2} - 49.250T^{-1}$
$\Delta Gf° = -53.463 + 2.557\times10^{-3}T\ln T + 0.466\times10^{-6}T^{2} - 24.625T^{-1} - 19.629\times10^{-3}T$
1363-2000 K: $\Delta Hf° = -87.320 - 1.516\times10^{-3}T + 0.608\times10^{-6}T^{2} + 214.350T^{-1}$
$\Delta Gf° = -87.320 + 1.516\times10^{-3}T\ln T - 0.608\times10^{-6}T^{2} + 107.175T^{-1} + 14.118\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$Mg(OH)_2(c)$
Magnesium Dihydroxide, Brucite
[Formation: $Mg(c) + O_2(g) + H_2(g) = Mg(OH)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	18.466	15.090	15.090	0	-221.100	-199.355	146.130
300	18.539	15.204	15.091	.034	-221.103	-199.220	145.129
400	21.925	21.036	15.863	2.069	-221.082	-191.922	104.860
500	23.866	26.160	17.422	4.369	-220.851	-184.657	80.713
600	24.924	30.613	19.256	6.814	-220.527	-177.443	64.633
700	25.616	34.510	21.164	9.342	-220.173	-170.291	53.167
800	26.244	37.971	23.052	11.935	-219.806	-163.193	44.582
900	26.982	41.103	24.886	14.595	-219.422	-156.134	37.914

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp° = 24.147 + 4.000\times10^{-3}T - 6.110\times10^{5}T^{-2}$

$H°-H°_{298} = 24.147\times10^{-3}T + 2.000\times10^{-6}T^{2} + 6.110\times10^{2}T^{-1} - 9.427$

Formation equations (kcal/mol):

298.15-900 K: $\Delta Hf° = -224.605 + 5.318\times10^{-3}T - 0.310\times10^{-6}T^{2} + 580.400T^{-1}$

$\Delta Gf° = -224.605 - 5.318\times10^{-3}T\ln T + 0.310\times10^{-6}T^{2} + 290.200T^{-1} + 111.630\times10^{-3}T$

Source: Data from King (265).

$Mg(OH)_2(g)$
Magnesium Dihydroxide (ideal gas)
[Formation: $Mg(c,l,g) + O_2(g) + H_2(g) = Mg(OH)_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.605	63.854	63.854	0	-136.800	-129.594	94.994
300	16.649	63.957	63.854	.031	-136.806	-129.548	94.375
400	18.443	69.016	64.531	1.794	-137.057	-127.089	69.437
500	19.500	73.254	65.864	3.695	-137.225	-124.578	54.453
600	20.181	76.874	67.406	5.681	-137.360	-122.033	44.450
700	20.676	80.024	68.988	7.725	-137.490	-119.468	37.299
800	21.081	82.812	70.544	9.814	-137.627	-116.887	31.932
900	21.440	85.316	72.049	11.940	-137.777	-114.281	27.751
922	21.513	85.835	72.372	12.412	-137.811	-113.710	26.953
922	21.513	85.835	72.372	12.412	-139.950	-113.710	26.953
1000	21.771	87.592	73.492	14.100	-140.079	-111.491	24.366
1100	22.080	89.681	74.869	16.293	-140.251	-108.625	21.582
1200	22.370	91.615	76.185	18.516	-140.442	-105.743	19.258
1300	22.639	93.417	77.443	20.766	-140.644	-102.832	17.287
1363	22.796	94.491	78.205	22.198	-140.781	-101.015	16.197
1363	22.796	94.491	78.205	22.198	-171.031	-101.015	16.197
1400	22.888	95.103	78.644	23.043	-170.971	-99.116	15.473
1500	23.117	96.691	79.796	25.343	-170.805	-93.993	13.695
1600	23.326	98.189	80.898	27.666	-170.633	-88.876	12.140
1700	23.517	99.609	81.957	30.008	-170.457	-83.771	10.769
1800	23.690	100.958	82.976	32.368	-170.278	-78.676	9.552
1900	23.848	102.243	83.956	34.746	-170.097	-73.590	8.465
2000	23.991	103.470	84.901	37.138	-169.916	-68.516	7.487

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.623 + 2.430\times10^{-3}T - 3.327\times10^{5}T^{-2}$

$H° - H°_{298} = 19.623\times10^{-3}T + 1.215\times10^{-6}T^{2} + 3.327\times10^{2}T^{-1} - 7.074$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -137.953 + 0.794\times10^{-3}T - 1.095\times10^{-6}T^{2} + 302.100T^{-1}$

$\Delta Gf° = -137.953 - 0.794\times10^{-3}T\ln T + 1.095\times10^{-6}T^{2} + 151.050T^{-1} + 30.532\times10^{-3}T$

922-1363 K: $\Delta Hf° = -139.276 - 0.072\times10^{-3}T - 0.781\times10^{-6}T^{2} + 40.400T^{-1}$

$\Delta Gf° = -139.276 + 0.072\times10^{-3}T\ln T + 0.781\times10^{-6}T^{2} + 20.200T^{-1} + 26.499\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -173.134 + 0.969\times10^{-3}T + 0.293\times10^{-6}T^{2} + 304.000T^{-1}$

$\Delta Gf° = -173.134 - 0.969\times10^{-3}T\ln T - 0.293\times10^{-6}T^{2} + 152.000T^{-1} + 60.246\times10^{-3}T$

Source: Data from Chase (82) who estimated all except enthalpy of formation at 298 K.

$Mg_3(PO_4)_2$(c,l)
Magnesium Phosphate
[Formation: $3Mg(c,l,g) + 2P(c,l,1/4P_4(g)) + 4O_2(g) = Mg_3(PO_4)_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	51.020	45.220	45.220	0	-903.600	-845.798	619.978
300	51.254	45.536	45.220	.095	-903.612	-845.436	615.892
317.3	52.845	48.454	45.317	.995	-903.707	-842.076	579.998
317.3	52.845	48.454	45.317	.995	-904.021	-842.076	579.998
400	60.451	61.726	47.369	5.743	-904.186	-825.908	451.249
500	65.640	75.813	51.681	12.066	-903.962	-806.361	352.456
550	67.479	82.170	54.166	15.402	-903.742	-796.629	316.547
550	67.479	82.170	54.166	15.402	-909.558	-796.629	316.547
600	69.318	88.121	56.751	18.822	-909.136	-786.380	286.435
700	72.248	99.034	62.027	25.905	-908.191	-765.991	239.150
800	74.747	108.848	67.276	33.258	-907.152	-745.760	203.730
900	76.968	117.782	72.399	40.845	-906.038	-725.635	176.206
922	77.413	119.646	73.504	42.543	-905.780	-721.240	170.960
922	77.413	119.646	73.504	42.543	-912.197	-721.240	170.960
1000	78.991	125.998	77.353	48.645	-911.267	-705.139	154.106
1100	80.861	133.615	82.125	56.639	-910.003	-684.592	136.014
1200	82.606	140.727	86.716	64.813	-908.689	-664.166	120.960
1300	84.243	147.404	91.130	73.156	-907.300	-643.808	108.233
1363	85.213	151.414	93.824	78.495	-906.405	-631.121	101.196
1363	85.213	151.414	93.824	78.495	-997.155	-631.121	101.196
1400	85.782	153.704	95.377	81.658	-996.188	-621.199	96.972
1500	87.233	159.672	99.465	90.310	-993.491	-594.513	86.619
1600	88.600	165.346	103.407	99.102	-990.682	-568.004	77.585
1626	88.942	166.777	104.410	101.410	-989.933	-561.141	75.422
1626	112.000	184.576	104.410	130.350	-960.993	-561.141	75.422
1700	112.000	189.560	108.008	138.638	-957.151	-543.029	69.810

Phase changes:
317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to P_4(g); ΔH° = 2.908 kcal/mol of P.
922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.
1626 K, melting point of $Mg_3(PO_4)_2$; ΔH° = 28.940 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1626 K: $Cp° = 64.368 + 15.926x10^{-3}T - 16.087x10^{5}T^{-2}$
$H° - H°_{298} = 64.368x10^{-3}T + 7.963x10^{-6}T^{2} + 16.087x10^{2}T^{-1} - 25.295$
1626-1700 K: $Cp° = 112.000$
$H° - H°_{298} = 112.000x10^{-3}T - 51.762$

Formation equations (kcal/mol):

298.15-317.3 K: $ΔHf° = -911.666 + 12.421x10^{-3}T - 4.583x10^{-6}T^{2} + 1422.200T^{-1}$
$ΔGf° = -911.666 - 12.421x10^{-3}TlnT + 4.583x10^{-6}T^{2} + 711.100T^{-1} + 282.327x10^{-3}T$
317.3-550 K: $ΔHf° = -911.039 + 7.435x10^{-3}T + 1.787x10^{-6}T^{2} + 1422.200T^{-1}$
$ΔGf° = -911.039 - 7.435x10^{-3}TlnT - 1.787x10^{-6}T^{2} + 711.100T^{-1} + 253.655x10^{-3}T$
550-922 K: $ΔHf° = -917.960 + 10.111x10^{-3}T + 1.779x10^{-6}T^{2} + 1221.600T^{-1}$
$ΔGf° = -917.960 - 10\ 111x10^{-3}TlnT - 1.779x10^{-6}T^{2} + 610.800T^{-1} + 283.451x10^{-3}T$
922-1363 K: $ΔHf° = -921.931 + 7.513x10^{-3}T + 2.721x10^{-6}T^{2} + 436.500T^{-1}$
$ΔGf° = -921.931 - 7.513x10^{-3}TlnT - 2.721x10^{-6}T^{2} + 218.250T^{-1} + 271.352x10^{-3}T$
1363-1626 K: $ΔHf° = -1023.503 + 10.636x10^{-3}T + 5.943x10^{-6}T^{2} + 1227.300T^{-1}$
$ΔGf° = -1023.503 - 10.636x10^{-3}TlnT - 5.943x10^{-6}T^{2} + 613.650T^{-1} + 372.592x10^{-3}T$
1626-1700 K: $ΔHf° = -1049.970 + 58.268x10^{-3}T - 2.020x10^{-6}T^{2} - 381.400T^{-1}$
$ΔGf° = -1049.970 - 58.268x10^{-3}TlnT + 2.020x10^{-6}T^{2} - 190.700T^{-1} + 728.412x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Other data based on Oetting (360).

$MgSO_4(\alpha,l)$
α-Magnesium Sulfate
[Reaction: $Mg(c,l,g) + 0.5S_2(g) + 2O_2(g) = MgSO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	23.000	21.844	21.844	0	-323.385	-290.222	212.736
300*	23.050	21.987	21.844	.043	-323.386	-290.014	211.273
400	26.290	29.085	22.790	2.518	-323.340	-278.893	152.378
500	28.540	35.199	24.675	5.262	-323.111	-267.806	117.057
600	30.500	40.581	26.886	8.217	-322.755	-256.773	93.528
700	32.100	45.404	29.193	11.348	-322.305	-245.809	76.744
800	33.580	49.788	31.497	14.633	-321.773	-234.921	64.177
900	34.950	53.823	33.756	18.060	-321.165	-224.095	54.417
922	35.236	54.671	34.245	18.832	-321.021	-221.728	52.557
922	35.236	54.671	34.245	18.832	-323.160	-221.728	52.557
1000	36.250	57.574	35.953	21.621	-322.619	-213.174	46.589
1100	37.450	61.086	38.081	25.306	-321.859	-202.269	40.187
1200	38.580	64.394	40.136	29.109	-321.034	-191.434	34.864
1300	39.520	67.520	42.123	33.016	-320.143	-180.657	30.371
1363	40.012	69.402	43.341	35.522	-319.563	-173.931	27.889
1363	40.012	69.402	43.341	35.522	-349.813	-173.931	27.889
1400	40.301	70.478	44.044	37.008	-349.321	-169.164	26.407
1400	38.000	73.034	44.044	40.586	-345.743	-169.164	26.407
1500	38.000	75.656	46.065	44.386	-344.643	-156.593	22.815
1600	38.000	78.108	47.992	48.186	-343.559	-144.090	19.682
1700	38.000	80.412	49.832	51.986	-342.490	-131.656	16.925
1800	38.000	82.584	51.592	55.786	-341.434	-119.282	14.483
1900	38.000	84.639	53.278	59.586	-340.394	-106.970	12.304
2000	38.000	86.588	54.895	63.386	-339.367	-94.711	10.349

*Data above 298 K estimated.

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.
1400 K, melting point of $MgSO_4$; ΔH° = 3.578 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 24.356 + 12.118\times10^{-3}T - 4.418\times10^{5}T^{-2}$
$H°-H°_{298} = 24.356\times10^{-3}T + 6.059\times10^{-6}T^2 + 4.418\times10^{2}T^{-1} - 9.282$
1400-2000 K: $Cp° = 38.000$
$H°-H°_{298} = 38.000\times10^{-3}T - 12.614$

Reaction equations (kcal/mol):

298.15-922 K: $\Delta Hr° = -324.928 + 0.581\times10^{-3}T + 3.505\times10^{-6}T^2 + 315.350T^{-1}$
$\Delta Gr° = -324.928 - 0.581\times10^{-3}T\ln T - 3.505\times10^{-6}T^2 + 157.675T^{-1} + 118.987\times10^{-3}T$
922-1363 K: $\Delta Hr° = -326.251 - 0.285\times10^{-3}T + 3.819\times10^{-6}T^2 + 53.650T^{-1}$
$\Delta Gr° = -326.251 + 0.285\times10^{-3}T\ln T - 3.819\times10^{-6}T^2 + 26.825T^{-1} + 114.955\times10^{-3}T$
1363-1400 K: $\Delta Hr° = -360.109 + 0.756\times10^{-3}T + 4.893\times10^{-6}T^2 + 317.250T^{-1}$
$\Delta Gr° = -360.109 - 0.756\times10^{-3}T\ln T - 4.893\times10^{-6}T^2 + 158.625T^{-1} + 148.701\times10^{-3}T$
1400-2000 K: $\Delta Hr° = -363.441 + 14.400\times10^{-3}T - 1.166\times10^{-6}T^2 - 124.550T^{-1}$
$\Delta Gr° = -363.441 - 14.400\times10^{-3}T\ln T + 1.166\times10^{-6}T^2 - 62.275T^{-1} + 241.552\times10^{-3}T$

Source: Data from DeKock (113). Data above 298 K estimated.

$MgSO_4(\beta,l)$
β-Magnesium Sulfate
[Reaction: $Mg(c,l,g) + 0.5S_2(g) + 2O_2(g) = MgSO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	23.000	21.844	21.844	0	-322.465	-289.302	212.061
300*	23.050	21.987	21.844	.043	-322.466	-289.094	210.602
400	26.290	29.085	22.790	2.518	-322.420	-277.973	151.875
500	28.540	35.199	24.675	5.262	-322.190	-266.886	116.654
600	30.500	40.581	26.886	8.217	-321.835	-255.853	93.193
700	32.100	45.404	29.193	11.348	-321.385	-244.889	76.457
800	33.580	49.788	31.497	14.633	-320.853	-234.001	63.925
900	34.950	53.823	33.756	18.060	-320.245	-223.175	54.194
922	35.236	54.671	34.245	18.832	-320.101	-220.808	52.339
922	35.236	54.671	34.245	18.832	-322.240	-220.808	52.339
1000	36.250	57.574	35.953	21.621	-321.699	-212.254	46.388
1100	37.450	61.086	38.081	25.306	-320.939	-201.349	40.004
1200	38.580	64.394	40.136	29.109	-320.113	-190.514	34.697
1300	39.520	67.520	42.123	33.016	-319.223	-179.737	30.216
1363	40.012	69.402	43.341	35.522	-318.643	-173.011	27.741
1363	40.012	69.402	43.341	35.522	-348.893	-173.011	27.741
1400	40.301	70.478	44.044	37.008	-348.401	-168.244	26.264
1400	38.000	73.034	44.044	40.586	-344.823	-168.244	26.264
1500	38.000	75.656	46.065	44.386	-343.723	-155.673	22.681
1600	38.000	78.108	47.992	48.186	-342.639	-143.170	19.556
1700	38.000	80.412	49.832	51.986	-341.569	-130.736	16.807
1800	38.000	82.584	51.592	55.786	-340.513	-118.362	14.371
1900	38.000	84.639	53.278	59.586	-339.474	-106.050	12.198
2000	38.000	86.588	54.895	63.386	-338.447	-93.791	10.249

*Data above 298 K estimated.

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.
1400 K, melting point of $MgSO_4$; ΔH° = 3.578 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp^\circ = 24.356 + 12.118\times10^{-3}T - 4.418\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 24.356\times10^{-3}T + 6.059\times10^{-6}T^{2} + 4.418\times10^{2}T^{-1} - 9.282$
1400.00-2000 K: $Cp^\circ = 38.000$
$H^\circ - H^\circ_{298} = 38.000\times10^{-3}T - 12.614$

Reaction equations (kcal/mol):

298.15-922 K: $\Delta Hr^\circ = -324.008 + 0.581\times10^{-3}T + 3.505\times10^{-6}T^{2} + 315.350T^{-1}$
$\Delta Gr^\circ = -324.008 - 0.581\times10^{-3}T\ln T - 3.505\times10^{-6}T^{2} + 157.675T^{-1} + 118.987\times10^{-3}T$
922-1363 K: $\Delta Hr^\circ = -325.331 - 0.285\times10^{-3}T + 3.819\times10^{-6}T^{2} + 53.650T^{-1}$
$\Delta Gr^\circ = -325.331 + 0.285\times10^{-3}T\ln T - 3.819\times10^{-6}T^{2} + 26.825T^{-1} + 114.955\times10^{-3}T$
1363-1400 K: $\Delta Hr^\circ = -359.189 + 0.756\times10^{-3}T + 4.893\times10^{-6}T^{2} + 317.250T^{-1}$
$\Delta Gr^\circ = -359.189 - 0.756\times10^{-3}T\ln T - 4.893\times10^{-6}T^{2} + 158.625T^{-1} + 148.701\times10^{-3}T$
1400-2000 K: $\Delta Hr^\circ = -362.521 + 14.400\times10^{-3}T - 1.166\times10^{-6}T^{2} - 124.550T^{-1}$
$\Delta Gr^\circ = -362.521 - 14.400\times10^{-3}T\ln T + 1.166\times10^{-6}T^{2} - 62.275T^{-1} + 241.552\times10^{-3}T$

Source: Data from DeKock (113). Data above 298 K estimated.

$MgSO_4 \cdot H_2O(c)$
Magnesium Sulfate Monohydrate
[Reaction: $Mg(c) + 0.5S_2(g) + 2.5O_2(g) + H_2(g) = MgSO_4 \cdot H_2O(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15*	34.600	30.200	30.200	0	-400.155	-352.874	258.660
300	34.767	30.415	30.202	.064	-400.154	-352.579	256.850
350	39.274	36.112	30.641	1.915	-400.030	-344.658	215.212
400	43.780	41.651	31.671	3.992	-399.704	-336.767	183.999
450	48.287	47.068	33.084	6.293	-399.181	-328.932	159.749
500	52.794	52.388	34.748	8.820	-398.455	-321.162	140.378
550	57.301	57.631	36.589	11.573	-397.529	-313.472	124.561

*Data except enthalpy of formation and entropy at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp^\circ = 7.587 + 90.382x10^{-3}T + 0.058x10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 7.587x10^{-3}T + 45.191x10^{-6}T^2 - 0.058x10^{2}T^{-1} - 6.260$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr^\circ = -395.593 - 26.259x10^{-3}T + 41.966x10^{-6}T^2 - 138.350T^{-1}$
$\Delta Gr^\circ = -395.593 + 26.259x10^{-3}T\ln T - 41.966x10^{-6}T^2 - 69.175T^{-1} + 6.960x10^{-3}T$

Source: Data from DeKock (113) who estimated all except enthalpy of formation and entropy at 298 K.

$MgSO_4 \cdot 2H_2O(c)$
Magnesium Sulfate Dihydrate
[Reaction: $Mg(c) + 0.5S_2(g) + 3O_2(g) + 2H_2(g) = MgSO_4 \cdot 2H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	42.000	40.000	40.000	0	-468.655	-407.686	298.838
300	42.185	40.260	40.000	.078	-468.660	-407.306	296.718
350	47.193	47.139	40.533	2.312	-468.675	-397.078	247.943
400	52.200	53.768	41.776	4.797	-468.468	-386.861	211.368
450	57.208	60.205	43.467	7.532	-468.041	-376.685	182.941
500	62.215	66.492	45.456	10.518	-467.390	-366.566	160.224
550	67.223	72.657	47.650	13.754	-466.518	-356.521	141.667

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 11.782 + 100.818 \times 10^{-3}T + 0.141 \times 10^{5}T^{-2}$
$H° - H°_{298} = 11.782 \times 10^{-3}T + 50.409 \times 10^{-6}T^{2} - 0.141 \times 10^{2}T^{-1} - 7.947$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -462.697 - 32.135 \times 10^{-3}T + 46.514 \times 10^{-6}T^{2} - 152.750T^{-1}$
$\Delta Gr° = -462.697 + 32.135 \times 10^{-3}T\ln T - 46.514 \times 10^{-6}T^{2} - 76.375T^{-1} + 16.145 \times 10^{-3}T$

Source: Data from DeKock (113) who estimated all except enthalpy of formation at 298 K.

$MgSO_4 \cdot 4H_2O(c)$
Magnesium Sulfate Tetrahydrate
[Reaction: $Mg(c) + 0.5S_2(g) + 4O_2(g) + 4H_2(g) = MgSO_4 \cdot 4H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	60.000	59.000	59.000	0	-612.155	-523.631	383.827
300	60.259	59.372	59.002	.111	-612.166	-523.081	381.059
350	67.270	69.187	59.761	3.299	-612.272	-508.221	317.344
400	74.280	78.628	61.533	6.838	-612.064	-493.367	269.560
450	81.291	87.781	63.941	10.728	-611.544	-478.559	232.417
500	88.301	96.709	66.775	14.967	-610.708	-463.825	202.735
550	95.312	105.454	69.894	19.558	-609.554	-449.187	178.488

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 18.542 + 139.592x10^{-3}T - 0.144x10^{5}T^{-2}$

$H°- H°_{298} = 18.542x10^{-3}T + 69.796x10^{-6}T^{2} + 0.144x10^{2}T^{-1} - 11.781$

Reaction equations (kcal/mol):

298.15-550 K: $ΔHr° = -603.866 - 45.517x10^{-3}T + 64.560x10^{-6}T^{2} - 136.450T^{-1}$

$ΔGr° = -603.866 + 45.517x10^{-3}T\ln T - 64.560x10^{-6}T^{2} - 68.225T^{-1} + 29.789x10^{-3}T$

Source: Data from DeKock (113) who estimated all except enthalpy of formation at 298 K.

$MgSO_4 \cdot 6H_2O(c)$
Magnesium Sulfate Hexahydrate
[Reaction: $Mg(c) + 0.5S_2(g) + 5O_2(g) + 6H_2(g) = MgSO_4 \cdot 6H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	83.200	83.200	83.200	0	-753.235	-638.707	468.179
300	83.573	83.716	83.203	.154	-753.242	-637.995	464.773
350*	93.090	97.327	84.256	4.575	-753.160	-618.788	386.384
400	101.520	110.320	86.708	9.445	-752.674	-599.620	327.613
450	108.864	122.712	90.025	14.709	-751.841	-580.538	281.944
500	115.121	134.516	93.890	20.313	-750.708	-561.562	245.456
550	120.291	145.739	98.097	26.203	-749.329	-542.709	215.650

*Data extrapolated above 320 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 71.180 + 100.386 \times 10^{-3}T - 15.921 \times 10^{5}T^{-2}$

$H° - H°_{298} = 71.180 \times 10^{-3}T + 50.193 \times 10^{-6}T^{2} + 15.921 \times 10^{2}T^{-1} - 31.024$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -758.023 - 13.021 \times 10^{-3}T + 43.616 \times 10^{-6}T^{2} + 1429.050T^{-1}$

$\Delta Gr° = -758.023 + 13.021 \times 10^{-3}T\ln T - 43.616 \times 10^{-6}T^{2} + 714.525T^{-1} + 330.970 \times 10^{-3}T$

Source: Data from DeKock (113) who extrapolated above 320 K.

$MgSO_4 \cdot 7H_2O(c)$
Magnesium Sulfate Heptahydrate

[Reaction: $Mg(c) + 0.5S_2(g) + 5.5O_2(g) + 7H_2(g) = MgSO_4 \cdot 7H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	91.000	89.000	89.000	0	-825.355	-695.946	510.136
300	91.463	89.564	89.001	.169	-825.367	-695.142	506.404
350	103.982	104.604	90.161	5.055	-825.342	-673.432	420.505
400	116.501	119.306	92.889	10.567	-824.740	-651.764	356.103
450	129.020	133.750	96.628	16.705	-823.564	-630.209	306.067
500	141.538	147.992	101.054	23.469	-821.805	-608.814	266.109
550	154.057	162.069	105.962	30.859	-819.463	-587.621	233.496

*Data except enthalpy of formation and entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 16.347 + 250.386 \times 10^{-3}T + 0.001 \times 10^{5}T^{-2}$

$H° - H°_{298} = 16.347 \times 10^{-3}T + 125.193 \times 10^{-6}T^{2} - 0.001 \times 10^{2}T^{-1} - 16.002$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -812.039 - 77.924 \times 10^{-3}T + 117.945 \times 10^{-6}T^{2} - 169.250T^{-1}$

$\Delta Gr° = -812.039 + 77.924 \times 10^{-3}T\ln T - 117.945 \times 10^{-6}T^{2} - 84.625T^{-1} - 18.489 \times 10^{-3}T$

Source: Data from DeKock (113) who estimated all except enthalpy of formation and entropy at 298 K.

Mg_2Si(c,l)
Dimagnesium Silicide
[Formation: 2Mg(c,l,g) + Si(c,l) = Mg_2Si(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ-H^\circ_{298})/T$	$H^\circ-H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	16.360	18.120	18.120	0	-18.600	-18.004	13.197
300*	16.386	18.221	18.121	.030	-18.601	-17.998	13.112
400	17.553	23.109	18.779	1.732	-18.626	-17.798	9.724
500	18.368	27.117	20.057	3.530	-18.652	-17.590	7.689
600	19.013	30.525	21.525	5.400	-18.686	-17.369	6.327
700	19.561	33.498	23.028	7.329	-18.736	-17.146	5.353
800	20.047	36.143	24.506	9.310	-18.804	-16.918	4.622
900	20.491	38.530	25.933	11.337	-18.899	-16.667	4.047
922	20.582	39.026	26.240	11.789	-18.921	-16.620	3.940
922	20.582	39.026	26.240	11.789	-23.199	-16.620	3.940
1000	20.905	40.710	27.303	13.407	-23.291	-16.061	3.510
1100	21.298	42.721	28.614	15.518	-23.417	-15.344	3.049
1200	21.674	44.591	29.869	17.666	-23.573	-14.610	2.661
1300	22.037	46.340	31.069	19.852	-23.737	-13.831	2.325
1363	22.260	47.388	31.799	21.248	-23.855	-13.383	2.146
1363	22.260	47.388	31.799	21.248	-84.355	-13.383	2.146
1375	22.302	47.583	31.936	21.515	-84.285	-12.763	2.029
1375	22.500	58.733	31.936	36.845	-68.955	-12.763	2.029
1400	22.500	59.138	32.419	37.407	-68.807	-11.740	1.833
1500	22.500	60.690	34.252	39.657	-68.214	-7.698	1.122
1600	22.500	62.142	35.950	41.907	-67.626	-3.684	.503
1687	22.500	63.334	37.333	43.865	-67.119	-.202	.026
1687	22.500	63.334	37.333	43.865	-79.201	-.202	.026
1700	22.500	63.507	37.532	44.157	-79.117	.411	-.053
1800	22.500	64.793	39.011	46.407	-78.469	5.074	-.616
1900	22.500	66.009	40.400	48.657	-77.823	9.700	-1.116
2000	22.500	67.163	41.710	50.907	-77.177	14.285	-1.561

*Data above 298 K except temperature and enthalpy of fusion estimated.

Phase changes:
922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.
1375 K, melting point of Mg_2Si; ΔH° = 15.330 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1375 K: $Cp^\circ = 17.113 + 3.926\times10^{-3}T - 1.711\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.113\times10^{-3}T + 1.963\times10^{-6}T^2 + 1.711\times10^{2}T^{-1} - 5.851$
1375-2000 K: $Cp^\circ = 22.500$
$H^\circ - H^\circ_{298} = 22.500\times10^{-3}T + 5.908$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf^\circ = -19.070 + 1.148\times10^{-3}T - 1.164\times10^{-6}T^2 + 68.800T^{-1}$
$\Delta Gf^\circ = -19.070 - 1.148\times10^{-3}T\ln T + 1.164\times10^{-6}T^2 + 34.400T^{-1} + 9.382\times10^{-3}T$
922-1363 K: $\Delta Hf^\circ = -21.717 - 0.584\times10^{-3}T - 0.536\times10^{-6}T^2 - 454.600T^{-1}$
$\Delta Gf^\circ = -21.717 + 0.584\times10^{-3}T\ln T + 0.536\times10^{-6}T^2 - 227.300T^{-1} + 1.316\times10^{-3}T$
1363-1375 K: $\Delta Hf^\circ = -89.432 + 1.498\times10^{-3}T + 1.612\times10^{-6}T^2 + 72.600T^{-1}$
$\Delta Gf^\circ = -89.432 - 1.498\times10^{-3}T\ln T - 1.612\times10^{-6}T^2 + 36.300T^{-1} + 68.810\times10^{-3}T$
1375-1687 K: $\Delta Hf^\circ = -77.673 + 6.885\times10^{-3}T - 0.351\times10^{-6}T^2 - 98.500T^{-1}$
$\Delta Gf^\circ = -77.673 - 6.885\times10^{-3}T\ln T + 0.351\times10^{-6}T^2 - 49.250T^{-1} + 96.532\times10^{-3}T$
1687-2000 K: $\Delta Hf^\circ = -90.102 + 6.464\times10^{-3}T$
$\Delta Gf^\circ = -90.102 - 6.464\times10^{-3}T\ln T + 101.346\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Gerstein (172). High-temperature data except temperature and enthalpy of fusion estimated.

$MgSiO_3$(enstatite)
Magnesium Silicate, Enstatite
[Formation: $Mg(c,l) + Si(c) + 1.5O_2(g) = MgSiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	20.600	19.524	19.524	0	-370.300	-350.535	256.945
300	20.665	19.652	19.525	.038	-370.301	-350.411	255.271
400	23.462	26.008	20.371	2.255	-370.266	-343.784	187.832
500	25.381	31.461	22.057	4.702	-370.101	-337.181	147.380
600	26.829	36.222	24.030	7.315	-369.858	-330.616	120.425
700	27.985	40.448	26.079	10.058	-369.567	-324.098	101.187
800	28.937	44.249	28.117	12.906	-369.243	-317.627	86.770
900	29.734	47.704	30.104	15.840	-368.901	-311.189	75.566
922	29.882	48.424	30.533	16.496	-368.823	-309.784	73.430
922	29.882	48.424	30.533	16.496	-370.962	-309.784	73.430
1000	30.406	50.873	32.025	18.848	-370.679	-304.617	66.573

Phase change: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 22.129 + 9.386 \times 10^{-3} T - 3.847 \times 10^{5} T^{-2}$
$H° - H°_{298} = 22.129 \times 10^{-3} T + 4.693 \times 10^{-6} T^{2} + 3.847 \times 10^{2} T^{-1} - 8.305$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -371.359 + 0.462 \times 10^{-3} T + 2.199 \times 10^{-6} T^{2} + 216.500 T^{-1}$
$\Delta Gf° = -371.359 - 0.462 \times 10^{-3} T \ln T - 2.199 \times 10^{-6} T^{2} + 108.250 T^{-1} + 71.917 \times 10^{-3} T$
922-1000 K: $\Delta Hf° = -372.683 - 0.404 \times 10^{-3} T + 2.513 \times 10^{-6} T^{2} - 45.200 T^{-1}$
$\Delta Gf° = -372.683 + 0.404 \times 10^{-3} T \ln T - 2.513 \times 10^{-6} T^{2} - 22.600 T^{-1} + 67.884 \times 10^{-3} T$

Sources: Enthalpy of formation at 298 K based on Charlu (75). Low-temperature heat capacities and entropy at 298 K from Krupka (286). High-temperature data based on Krupka (285).

Mg_2SiO_4(forsterite)

Dimagnesium Silicate, Forsterite

[Formation: $2Mg(c,l,g) + Si(c,l) + 2O_2(g) = Mg_2SiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	28.350	22.493	22.493	0	-519.620	-491.106	359.986
300	28.464	22.669	22.493	.053	-519.624	-490.926	357.635
400	32.806	31.513	23.670	3.137	-519.687	-481.348	262.993
500	35.405	39.132	26.018	6.557	-519.553	-471.778	206.211
600	37.258	45.759	28.769	10.194	-519.330	-462.237	168.368
700	38.720	51.616	31.623	13.995	-519.064	-452.742	141.351
800	39.939	56.868	34.456	17.930	-518.774	-443.292	121.100
900	40.986	61.634	37.215	21.977	-518.477	-433.864	105.355
922	41.187	62.626	37.810	22.881	-518.408	-431.805	102.353
922	41.187	62.626	37.810	22.881	-522.686	-431.805	102.353
1000	41.899	66.000	39.877	26.123	-522.447	-424.127	92.692
1100	42.698	70.032	42.438	30.353	-522.132	-414.323	82.317
1200	43.397	73.778	44.896	34.659	-521.826	-404.540	73.676
1300	44.003	77.276	47.253	39.030	-521.517	-394.754	66.363
1363	44.330	79.367	48.690	41.813	-521.334	-388.652	62.317
1363	44.330	79.367	48.690	41.813	-581.834	-388.652	62.317
1400	44.522	80.557	49.516	43.457	-581.443	-383.414	59.853
1500	44.958	83.644	51.690	47.931	-580.366	-369.322	53.809
1600	45.312	86.557	53.778	52.446	-579.267	-355.288	48.529
1687	45.551	88.963	55.532	56.399	-578.299	-343.115	44.450
1687	45.551	88.963	55.532	56.399	-590.381	-343.115	44.450
1700	45.587	89.313	55.789	56.991	-590.227	-341.206	43.864
1800	45.783	91.924	57.724	61.560	-589.036	-326.585	39.652
1900	45.903	94.403	59.590	66.145	-587.843	-312.037	35.892
2000	45.946	96.759	61.390	70.738	-586.652	-297.558	32.515

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 36.480 + 5.786\times10^{-3}T - 8.761\times10^{5}T^{-2}$
$H°-H°_{298} = 36.480\times10^{-3}T + 2.893\times10^{-6}T^{2} + 8.761\times10^{2}T^{-1} - 14.072$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -523.607 + 6.055\times10^{-3}T - 1.240\times10^{-6}T^{2} + 683.400T^{-1}$
$\Delta Gf° = -523.607 - 6.055\times10^{-3}T\ln T + 1.240\times10^{-6}T^{2} + 341.700T^{-1} + 139.295\times10^{-3}T$
922-1363 K: $\Delta Hf° = -526.254 + 4.323\times10^{-3}T - 0.612\times10^{-6}T^{2} + 160.000T^{-1}$
$\Delta Gf° = -526.254 - 4.323\times10^{-3}T\ln T + 0.612\times10^{-6}T^{2} + 80.000T^{-1} + 131.230\times10^{-3}T$
1363-1687 K: $\Delta Hf° = -593.969 + 6.405\times10^{-3}T + 1.536\times10^{-6}T^{2} + 687.200T^{-1}$
$\Delta Gf° = -593.969 - 6.405\times10^{-3}T\ln T - 1.536\times10^{-6}T^{2} + 343.600T^{-1} + 198.723\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -606.399 + 5.984\times10^{-3}T + 1.887\times10^{-6}T^{2} + 785.700T^{-1}$
$\Delta Gf° = -606.399 - 5.984\times10^{-3}T\ln T - 1.887\times10^{-6}T^{2} + 392.850T^{-1} + 203.537\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Charlu (75). Low-temperature heat capacities and entropy at 298 K from Robie (427). High-temperature data based on Orr (375).

$MgTiO_3$(c)
Magnesium Titanate
[Formation: Mg(c,l,g) + Ti(c) + $1.5O_2$(g) = $MgTiO_3$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	21.940	21.930	21.930	0	-375.800	-355.911	260.887
300	22.030	22.066	21.930	.041	-375.801	-355.785	259.186
400	25.540	28.978	22.851	2.451	-375.681	-349.127	190.751
500	27.260	34.879	24.681	5.099	-375.412	-342.521	149.714
600	28.358	39.952	26.814	7.883	-375.090	-335.968	122.375
700	29.163	44.386	29.013	10.761	-374.763	-329.467	102.863
800	29.811	48.324	31.187	13.710	-374.445	-323.025	88.245
900	30.368	51.868	33.290	16.720	-374.145	-316.608	76.882
922	30.478	52.603	33.742	17.389	-374.081	-315.206	74.715
922	30.478	52.603	33.742	17.389	-376.220	-315.206	74.715
1000	30.869	55.094	35.312	19.782	-375.999	-310.058	67.762
1100	31.332	58.058	37.247	22.892	-375.730	-303.486	60.296
1156	31.578	59.621	38.294	24.654	-375.590	-299.810	56.680
1156	31.578	59.621	38.294	24.654	-376.607	-299.810	56.680
1200	31.771	60.804	39.097	26.048	-376.451	-296.890	54.070
1300	32.192	63.363	40.866	29.246	-376.108	-290.261	48.797
1363	32.449	64.893	41.942	31.283	-375.902	-286.126	45.878
1363	32.449	64.893	41.942	31.283	-406.152	-286.126	45.878
1400	32.600	65.764	42.560	32.486	-405.889	-282.872	44.158
1500	32.998	68.027	44.183	35.766	-405.172	-274.111	39.937
1600	33.389	70.169	45.741	39.085	-404.447	-265.398	36.251
1700	33.775	72.205	47.239	42.443	-403.715	-256.730	33.004
1800	34.156	74.146	48.679	45.840	-402.982	-248.103	30.123

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 27.888 + 3.586\times10^{-3}T - 6.052\times10^{5}T^{-2}$
$H°-H°_{298} = 27.888\times10^{-3}T + 1.793\times10^{-6}T^{2} + 6.052\times10^{2}T^{-1} - 10.504$

Formation equations (kcal/mol):

298.15-922 K: $ΔHf° = -379.331 + 6.423\times10^{-3}T - 1.472\times10^{-6}T^{2} + 520.700T^{-1}$
$ΔGf° = -379.331 - 6.423\times10^{-3}T\ln T + 1.472\times10^{-6}T^{2} + 260.350T^{-1} + 111.777\times10^{-3}T$
922-1156 K: $ΔHf° = -380.654 + 5.557\times10^{-3}T - 1.159\times10^{-6}T^{2} + 259.000T^{-1}$
$ΔGf° = -380.654 - 5.557\times10^{-3}T\ln T + 1.159\times10^{-6}T^{2} + 129.500T^{-1} + 107.744\times10^{-3}T$
1156-1363 K: $ΔHf° = -384.691 + 7.957\times10^{-3}T - 1.481\times10^{-6}T^{2} + 1041.900T^{-1}$
$ΔGf° = -384.691 - 7.957\times10^{-3}T\ln T + 1.481\times10^{-6}T^{2} + 520.950T^{-1} + 127.497\times10^{-3}T$
1363-1800 K: $ΔHf° = -418.549 + 8.998\times10^{-3}T - 0.407\times10^{-6}T^{2} + 1305.500T^{-1}$
$ΔGf° = -418.549 - 8.998\times10^{-3}T\ln T + 0.407\times10^{-6}T^{2} + 652.750T^{-1} + 161.243\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kelley (249). Low-temperature heat capacities and entropy at 298 K from Shomate (452). High-temperature data based on Naylor (353).

$MgTi_2O_5$(c)
Magnesium Dititanate
[Formation: $Mg(c,l,g) + 2Ti(c) + 2.5O_2(g) = MgTi_2O_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	35.150	30.410	30.410	0	-599.600	-565.446	414.478
300	35.265	30.628	30.411	.065	-599.600	-565.231	411.765
400	39.759	41.475	31.860	3.846	-599.436	-553.792	302.574
500	42.298	50.640	34.724	7.958	-599.077	-542.426	237.091
600	44.106	58.519	38.049	12.282	-598.635	-531.132	193.462
700	45.568	65.430	41.476	16.768	-598.165	-519.905	162.320
800	46.847	71.600	44.862	21.390	-597.686	-508.766	138.987
900	48.019	77.187	48.149	26.134	-597.205	-497.673	120.850
922	48.262	78.350	48.856	27.193	-597.096	-495.245	117.391
922	48.262	78.350	48.856	27.193	-599.235	-495.245	117.391
1000	49.124	82.303	51.312	30.991	-598.848	-486.466	106.316
1100	50.186	87.036	54.348	35.957	-598.346	-475.268	94.426
1156	50.764	89.542	55.993	38.783	-598.062	-469.004	88.667
1156	50.764	89.542	55.993	38.783	-600.096	-469.004	88.667
1200	51.218	91.447	57.258	41.027	-599.776	-464.021	84.509
1300	52.230	95.586	60.048	46.200	-599.034	-452.724	76.109
1363	52.857	98.073	61.749	49.510	-598.562	-445.667	71.459
1363	52.857	98.073	61.749	49.510	-628.812	-445.667	71.459
1400	53.226	99.494	62.728	51.473	-628.387	-440.701	68.796
1500	54.211	103.200	65.303	56.845	-627.208	-427.336	62.262
1600	55.188	106.729	67.782	62.315	-625.991	-414.051	56.556
1700	56.158	110.104	70.173	67.882	-624.738	-400.841	51.531
1800	57.123	113.342	72.483	73.546	-623.462	-387.709	47.074

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 40.451 + 9.384 \times 10^{-3}T - 7.113 \times 10^{5}T^{-2}$
$H° - H°_{298} = 40.451 \times 10^{-3}T + 4.692 \times 10^{-6}T^{2} + 7.113 \times 10^{2}T^{-1} - 14.863$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -603.355 + 6.279 \times 10^{-3}T - 0.200 \times 10^{-6}T^{2} + 566.800T^{-1}$
$\Delta Gf° = -603.355 - 6.279 \times 10^{-3}T\ln T + 0.200 \times 10^{-6}T^{2} + 283.400T^{-1} + 159.676 \times 10^{-3}T$
922-1156 K: $\Delta Hf° = -604.679 + 5.413 \times 10^{-3}T + 0.114 \times 10^{-6}T^{2} + 305.100T^{-1}$
$\Delta Gf° = -604.679 - 5.413 \times 10^{-3}T\ln T - 0.114 \times 10^{-6}T^{2} + 152.550T^{-1} + 155.643 \times 10^{-3}T$
1156-1363 K: $\Delta Hf° = -612.753 + 10.213 \times 10^{-3}T - 0.532 \times 10^{-6}T^{2} + 1870.900T^{-1}$
$\Delta Gf° = -612.753 - 10.213 \times 10^{-3}T\ln T + 0.532 \times 10^{-6}T^{2} + 935.450T^{-1} + 195.148 \times 10^{-3}T$
1363-1800 K: $\Delta Hf° = -646.610 + 11.254 \times 10^{-3}T + 0.542 \times 10^{-6}T^{2} + 2134.500T^{-1}$
$\Delta Gf° = -646.610 - 11.254 \times 10^{-3}T\ln T - 0.542 \times 10^{-6}T^{2} + 1067.250T^{-1} + 228.894 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kelley (249). Low-temperature heat capacities and entropy at 298 K from Todd (495). High-temperature data based on Orr (376).

$Mg_2TiO_4(c)$
Dimagnesium Titanate
[Formation: $2Mg(c,l,g) + Ti(c) + 2O_2(g) = Mg_2TiO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	30.750	26.130	26.130	0	-517.300	-489.029	358.464
300	30.857	26.321	26.131	.057	-517.302	-488.851	356.123
400	35.005	35.845	27.403	3.377	-517.238	-479.372	261.913
500	37.364	43.928	29.920	7.004	-516.994	-469.937	205.407
600	39.055	50.896	32.848	10.829	-516.675	-460.546	167.752
700	40.431	57.023	35.873	14.805	-516.332	-451.212	140.873
800	41.638	62.502	38.866	18.909	-515.981	-441.943	120.732
900	42.748	67.471	41.772	23.129	-515.629	-432.697	105.072
922	42.979	68.506	42.398	24.072	-515.549	-430.679	102.086
922	42.979	68.506	42.398	24.072	-519.827	-430.679	102.086
1000	43.797	72.030	44.573	27.457	-519.547	-423.157	92.480
1100	44.807	76.252	47.264	31.887	-519.178	-413.547	82.163
1156	45.357	78.491	48.723	34.412	-518.975	-408.176	77.167
1156	45.357	78.491	48.723	34.412	-519.992	-408.176	77.167
1200	45.789	80.193	49.846	36.417	-519.779	-403.924	73.564
1300	46.753	83.896	52.324	41.044	-519.285	-394.264	66.281
1363	47.351	86.122	53.834	44.009	-518.972	-388.252	62.253
1363	47.351	86.122	53.834	44.009	-579.472	-388.252	62.253
1400	47.702	87.395	54.704	45.767	-578.999	-383.069	59.799
1500	48.642	90.719	56.996	50.585	-577.675	-369.122	53.780
1600	49.573	93.888	59.204	55.495	-576.295	-355.265	48.526
1700	50.499	96.921	61.333	60.499	-574.855	-341.493	43.901
1800	51.420	99.833	63.391	65.595	-573.363	-327.805	39.800

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 35.479 + 8.968\times10^{-3}T - 6.498\times10^{5}T^{-2}$
$H°-H°_{298} = 35.479\times10^{-3}T + 4.484\times10^{-6}T^{2} + 6.498\times10^{2}T^{-1} - 13.156$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -520.643 + 5.256\times10^{-3}T - 0.421\times10^{-6}T^{2} + 540.800T^{-1}$
$\Delta Gf° = -520.643 - 5.256\times10^{-3}T\ln T + 0.421\times10^{-6}T^{2} + 270.400T^{-1} + 132.813\times10^{-3}T$
922-1156 K: $\Delta Hf° = -523.291 + 3.524\times10^{-3}T + 0.207\times10^{-6}T^{2} + 17.400T^{-1}$
$\Delta Gf° = -523.291 - 3.524\times10^{-3}T\ln T - 0.207\times10^{-6}T^{2} + 8.700T^{-1} + 124.748\times10^{-3}T$
1156-1363 K: $\Delta Hf° = -527.328 + 5.924\times10^{-3}T - 0.116\times10^{-6}T^{2} + 800.300T^{-1}$
$\Delta Gf° = -527.328 - 5.924\times10^{-3}T\ln T + 0.116\times10^{-6}T^{2} + 400.150T^{-1} + 144.500\times10^{-3}T$
1363-1800 K: $\Delta Hf° = -595.043 + 8.006\times10^{-3}T + 2.032\times10^{-6}T^{2} + 1327.500T^{-1}$
$\Delta Gf° = -595.043 - 8.006\times10^{-3}T\ln T - 2.032\times10^{-6}T^{2} + 663.750T^{-1} + 211.994\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kelley (249). Low-temperature heat capacities from Todd (495). Entropy at 298 K from Parker (391). High-temperature data based on Orr (376).

$MgUO_4(c)$
Magnesium Uranate

[Formation: $Mg(c,l,g) + U(c) + 2O_2(g) = MgUO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	30.617	31.525	31.525	0	-443.830	-418.101	306.472
300	30.641	31.714	31.525	.057	-443.822	-417.939	304.465
400	31.845	40.696	32.743	3.181	-443.414	-409.377	223.670
500	32.937	47.923	35.079	6.422	-443.010	-400.915	175.238
600	33.917	54.015	37.738	9.766	-442.639	-392.527	142.976
700	34.785	59.309	40.452	13.200	-442.323	-384.201	119.951
800	35.543	64.006	43.108	16.718	-442.076	-375.922	102.696
900	36.186	68.231	45.669	20.306	-441.916	-367.656	89.278
922	36.303	69.106	46.218	21.103	-441.894	-365.846	86.719
922	36.303	69.106	46.218	21.103	-444.033	-365.846	86.719
942	36.409	69.887	46.712	21.831	-444.017	-364.150	84.484
942	36.409	69.887	46.712	21.831	-444.684	-364.150	84.484
1000	36.718	72.072	48.119	23.953	-444.575	-359.199	78.502
1049	36.923	73.833	49.279	25.757	-444.481	-355.017	73.964
1049	36.923	73.833	49.279	25.757	-445.618	-355.017	73.964
1100	37.137	75.590	50.457	27.646	-445.466	-350.616	69.660
1200	37.445	78.836	52.688	31.377	-445.176	-342.008	62.287
1300	37.641	81.843	54.819	35.131	-444.899	-333.414	56.051
1363	37.694	83.627	56.110	37.506	-444.738	-328.034	52.598
1363	37.694	83.627	56.110	37.506	-474.988	-328.034	52.598
1400	37.725	84.637	56.851	38.901	-474.756	-324.049	50.586

Phase changes:
922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K:
$Cp° = 31.433 + 5.150\times10^{-3}T - 2.090\times10^{5}T^{-2}$
$H°-H°_{298} = 31.433\times10^{-3}T + 2.575\times10^{-6}T^{2} + 2.090\times10^{2}T^{-1} - 10.302$

Formation equations (kcal/mol):

298.15-922 K:
$ΔHf° = -446.755 + 8.720\times10^{-3}T - 4.041\times10^{-6}T^{2} + 204.200T^{-1}$
$ΔGf° = -446.755 - 8.720\times10^{-3}T\ln T + 4.041\times10^{-6}T^{2} + 102.100T^{-1} + 143.437\times10^{-3}T$

922-942 K:
$ΔHf° = -448.079 + 7.854\times10^{-3}T - 3.727\times10^{-6}T^{2} - 57.500T^{-1}$
$ΔGf° = -448.079 - 7.854\times10^{-3}T\ln T + 3.727\times10^{-6}T^{2} - 28.750T^{-1} + 139.404\times10^{-3}T$

942-1049 K:
$ΔHf° = -445.669 + 0.709\times10^{-3}T + 0.495\times10^{-6}T^{2} - 145.000T^{-1}$
$ΔGf° = -445.669 - 0.709\times10^{-3}T\ln T - 0.495\times10^{-6}T^{2} - 72.500T^{-1} + 91.943\times10^{-3}T$

1049-1363 K:
$ΔHf° = -447.965 + 1.814\times10^{-3}T + 0.495\times10^{-6}T^{2} - 145.000T^{-1}$
$ΔGf° = -447.965 - 1.814\times10^{-3}T\ln T - 0.495\times10^{-6}T^{2} - 72.500T^{-1} + 101.818\times10^{-3}T$

1363-1400 K:
$ΔHf° = -481.823 + 2.855\times10^{-3}T + 1.569\times10^{-6}T^{2} + 118.600T^{-1}$
$ΔGf° = -481.823 - 2.855\times10^{-3}T\ln T - 1.569\times10^{-6}T^{2} + 59.300T^{-1} + 135.565\times10^{-3}T$

Source: Data from O'Hare (366).

$MgWO_4(c)$
Magnesium Tungstate
[Formation: $Mg(c,l,g) + W(c) + 2O_2(g) = MgWO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	26.070	24.184	24.184	0	-366.300	-339.635	248.956
300*	26.200	24.346	24.186	.048	-366.300	-339.467	247.299
400	29.500	32.367	25.255	2.845	-366.124	-330.543	180.598
500	31.450	39.171	27.375	5.898	-365.778	-321.687	140.608
600	32.750	45.023	29.841	9.109	-365.361	-312.908	113.975
700	33.860	50.156	32.385	12.440	-364.906	-304.198	94.974
800	34.930	54.747	34.897	15.880	-364.416	-295.566	80.744
900	35.950	58.920	37.338	19.424	-363.892	-286.980	69.687
922	36.181	59.791	37.863	20.217	-363.770	-285.105	67.580
922	36.181	59.791	37.863	20.217	-365.909	-285.105	67.580
1000	37.000	62.762	39.691	23.071	-365.461	-278.293	60.820
1100	38.100	66.340	41.953	26.826	-364.837	-269.599	53.564
1200	39.200	69.702	44.126	30.691	-364.160	-260.979	47.530
1300	40.300	72.884	46.218	34.666	-363.416	-252.393	42.431
1363	40.961	74.806	47.494	37.225	-362.921	-247.035	39.610
1363	40.961	74.806	47.494	37.225	-393.171	-247.035	39.610
1400	41.350	75.908	48.231	38.748	-392.725	-243.075	37.945
1500	42.450	78.799	50.173	42.939	-391.457	-232.436	33.865
1600	43.500	81.572	52.049	47.236	-390.106	-221.876	30.306
1700	44.600	84.242	53.865	51.641	-388.664	-211.396	27.177
1800	45.650	86.821	55.625	56.153	-387.135	-201.022	24.407
1900	46.750	89.319	57.333	60.774	-385.517	-190.723	21.938
2000	47.800	91.744	58.993	65.502	-383.811	-180.521	19.726

*Data above 298 K estimated.

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 28.276 + 9.452\times10^{-3}T - 4.466\times10^{5}T^{-2}$

$H° - H°_{298} = 28.276\times10^{-3}T + 4.726\times10^{-6}T^{2} + 4.466\times10^{2}T^{-1} - 10.349$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -368.444 + 2.858\times10^{-3}T + 1.961\times10^{-6}T^{2} + 333.300T^{-1}$

$\Delta Gf° = -368.444 - 2.858\times10^{-3}T\ln T - 1.961\times10^{-6}T^{2} + 166.650T^{-1} + 111.622\times10^{-3}T$

922-1363 K: $\Delta Hf° = -369.768 + 1.992\times10^{-3}T + 2.275\times10^{-6}T^{2} + 71.600T^{-1}$

$\Delta Gf° = -369.768 - 1.992\times10^{-3}T\ln T - 2.275\times10^{-6}T^{2} + 35.800T^{-1} + 107.589\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -403.625 + 3.033\times10^{-3}T + 3.349\times10^{-6}T^{2} + 335.200T^{-1}$

$\Delta Gf° = -403.625 - 3.033\times10^{-3}T\ln T - 3.349\times10^{-6}T^{2} + 167.600T^{-1} + 141.336\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391) Other data from JANAF (127) who estimated all above 298 K.

MnAs(c)
Manganese Arsenide

[Formation: $Mn(c) + As[\alpha, 1/4As_4(g)] = MnAs(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	16.771	18.420	18.420	0	-14.000	-14.667	10.751
300	16.950	18.530	18.427	.031	-13.992	-14.673	10.689
316	311.000	19.810	18.560	.395	-13.824	-14.745	10.197
320	15.399	20.411	18.470	.621	-13.647	-14.722	10.055
340	13.640	21.243	18.614	.894	-13.622	-14.792	9.508
360	13.731	22.020	18.787	1.164	-13.603	-14.864	9.024
380	13.870	22.761	18.969	1.441	-13.579	-14.932	8.588
394	14.340	23.250	19.126	1.625	-13.573	-14.987	8.313
400	13.370	23.480	19.185	1.718	-13.557	-15.007	8.199
450	13.014	25.034	19.761	2.373	-13.550	-15.191	7.378
500	13.069	26.386	20.334	3.026	-13.560	-15.361	6.714
550	13.191	27.629	20.936	3.681	-13.583	-15.539	6.174
600	13.351	28.800	21.558	4.345	-13.610	-15.724	5.728
650	13.489	29.876	22.162	5.014	-13.646	-15.906	5.348
700	13.630	30.880	22.747	5.693	-13.684	-16.077	5.019

Phase changes: 316 K, second-order transition point of MnAs; ΔH° = 0 kcal/mol.
394 K, second-order transition point of MnAs; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-316 K: $Cp^\circ = -164.279 + 607.042\times10^{-3}T$
$H^\circ - H^\circ_{298} = -164.279\times10^{-3}T + 303.521\times10^{-6}T^2 + 21.999$
316-394 K: $Cp^\circ = 67.462 - 145.626\times10^{-3}T$
$H^\circ - H^\circ_{298} = 67.462\times10^{-3}T - 72.813\times10^{-6}T^2 - 13.652$
394-700 K: $Cp^\circ = -4.907 + 22.654\times10^{-3}T + 16.021\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = -4.907\times10^{-3}T + 11.327\times10^{-6}T^2 - 16.021\times10^{2}T^{-1} + 5.866$

Formation equations (kcal/mol):

298.15-316 K: $\Delta Hf^\circ = 11.733 - 175.608\times10^{-3}T + 301.243\times10^{-6}T^2 - 45.800T^{-1}$
$\Delta Gf^\circ = 11.733 + 175.608\times10^{-3}T\ln T - 301.243\times10^{-6}T^2 - 22.900T^{-1} - 999.014\times10^{-3}T$
316-394 K: $\Delta Hf^\circ = -23.918 + 56.133\times10^{-3}T - 75.091\times10^{-6}T^2 - 45.800T^{-1}$
$\Delta Gf^\circ = -23.918 - 56.133\times10^{-3}T\ln T + 75.091\times10^{-6}T^2 - 22.900T^{-1} + 328.725\times10^{-3}T$
394-700 K: $\Delta Hf^\circ = -4.400 - 16.236\times10^{-3}T + 9.049\times10^{-6}T^2 - 1647.900T^{-1}$
$\Delta Gf^\circ = -4.400 + 16.236\times10^{-3}T\ln T - 9.049\times10^{-6}T^2 - 823.950T^{-1} - 115.004\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Other data from Gronvold (190).

MnB(c)
Manganese Boride
[Formation: Mn(c,l) + B(β) = MnB(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.570	8.600	8.600	0	-17.400	-17.263	12.654
300	8.610	8.660	8.600	.020	-17.397	-17.259	12.573
400	10.160	11.370	8.970	.960	-17.426	-17.218	9.407
500	11.090	13.740	9.680	2.030	-17.461	-17.151	7.497
600	11.770	15.830	10.547	3.170	-17.538	-17.094	6.226
700	12.320	17.690	11.433	4.380	-17.628	-17.012	5.311
800	12.820	19.360	12.310	5.640	-17.732	-16.908	4.619
900	13.280	20.900	13.189	6.940	-17.851	-16.807	4.081
980	13.632	22.044	13.864	8.016	-17.944	-16.705	3.725
980	13.632	22.044	13.864	8.016	-18.476	-16.705	3.725
1000	13.720	22.320	14.030	8.290	-18.501	-16.671	3.643
1100	14.140	23.650	14.850	9.680	-18.620	-16.486	3.275
1200	14.550	24.900	15.633	11.120	-18.715	-16.291	2.967
1300	14.960	26.080	16.395	12.590	-18.805	-16.088	2.705
1360	15.200	26.757	16.831	13.499	-18.844	-15.944	2.562
1360	15.200	26.757	16.831	13.499	-19.351	-15.944	2.562
1400	15.360	27.200	17.121	14.110	-19.415	-15.845	2.473
1410	15.399	27.309	17.193	14.264	-19.431	-15.810	2.451
1410	15.399	27.309	17.193	14.264	-19.880	-15.810	2.451
1500	15.750	28.280	17.840	15.660	-20.062	-15.562	2.267
1517	15.818	28.458	17.958	15.928	-20.095	-15.502	2.233
1517	15.818	28.458	17.958	15.928	-22.977	-15.502	2.233
1600	16.150	29.300	18.512	17.260	-23.122	-15.074	2.059
1700	16.540	30.300	19.188	18.890	-23.284	-14.580	1.874
1800	16.930	31.250	19.822	20.570	-23.410	-14.032	1.704
1900	17.310	32.180	20.454	22.280	-23.520	-13.526	1.556
2000	17.700	33.080	21.065	24.030	-23.604	-13.004	1.421

*Data estimated.

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2100 K: $Cp° = 10.158 + 3.802\times10^{-3}T - 2.424\times10^{5}T^{-2}$
$H° - H°_{298} = 10.158\times10^{-3}T + 1.901\times10^{-6}T^{2} + 2.424\times10^{2}T^{-1} - 4.011$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = -17.253 - 0.203\times10^{-3}T - 0.498\times10^{-6}T^{2} - 12.500T^{-1}$
$\Delta Gf° = -17.253 + 0.203\times10^{-3}T\ln T + 0.498\times10^{-6}T^{2} - 6.250T^{-1} - 1.267\times10^{-3}T$
980-1360 K: $\Delta Hf° = -16.834 - 2.384\times10^{-3}T + 0.645\times10^{-6}T^{2} + 74.300T^{-1}$
$\Delta Gf° = -16.834 + 2.384\times10^{-3}T\ln T - 0.645\times10^{-6}T^{2} + 37.150T^{-1} - 15.641\times10^{-3}T$
1360-1410 K: $\Delta Hf° = -16.807 - 2.155\times10^{-3}T + 0.209\times10^{-6}T^{2} + 20.900T^{-1}$
$\Delta Gf° = -16.807 + 2.155\times10^{-3}T\ln T - 0.209\times10^{-6}T^{2} + 10.450T^{-1} - 14.588\times10^{-3}T$
1410-1517 K: $\Delta Hf° = -16.555 - 2.744\times10^{-3}T + 0.274\times10^{-6}T^{2} + 20.900T^{-1}$
$\Delta Gf° = -16.555 + 2.744\times10^{-3}T\ln T - 0.274\times10^{-6}T^{2} + 10.450T^{-1} - 18.946\times10^{-3}T$
1517-2000 K: $\Delta Hf° = -17.309 - 5.565\times10^{-3}T + 1.209\times10^{-6}T^{2} + 20.900T^{-1}$
$\Delta Gf° = -17.309 + 5.565\times10^{-3}T\ln T - 1.209\times10^{-6}T^{2} + 10.450T^{-1} - 37.693\times10^{-3}T$

Source: Data are those estimated by Hack (199).

$MnB_2(c)$
Manganese Diboride
[Formation: $Mn(c,l) + 2B(\beta) = MnB_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°$_{298}$)/T	H°- H°$_{298}$	ΔHf°	ΔGf°	
298.15*	9.880	10.610	10.610	0	-22.500	-22.542	16.523
300	9.970	10.670	10.610	.020	-22.502	-22.538	16.419
400	13.290	14.050	11.050	1.200	-22.608	-22.540	12.315
500	15.040	17.230	11.970	2.630	-22.690	-22.505	9.837
600	16.180	20.080	13.097	4.190	-22.822	-22.468	8.184
700	17.030	22.640	14.283	5.850	-22.980	-22.399	6.993
800	17.720	24.960	15.472	7.590	-23.150	-22.302	6.093
900	18.330	27.080	16.647	9.390	-23.338	-22.186	5.387
980	18.762	28.660	17.554	10.884	-23.483	-22.063	4.920
980	18.762	28.660	17.554	10.884	-24.015	-22.063	4.920
1000	18.870	29.040	17.780	11.260	-24.056	-22.026	4.814
1100	19.380	30.860	18.887	13.170	-24.259	-21.817	4.335
1200	19.870	32.570	19.962	15.130	-24.453	-21.597	3.933
1300	20.330	34.180	20.995	17.140	-24.637	-21.348	3.589
1360	20.606	35.100	21.591	18.372	-24.740	-21.176	3.403
1360	20.606	35.100	21.591	18.372	-25.247	-21.176	3.403
1400	20.790	35.700	21.986	19.200	-25.355	-21.057	3.287
1410	20.835	35.848	22.084	19.408	-25.382	-21.017	3.258
1410	20.835	35.848	22.084	19.408	-25.831	-21.017	3.258
1500	21.240	37.150	22.950	21.300	-26.115	-20.700	3.016
1517	21.313	37.390	23.110	21.662	-26.169	-20.629	2.972
1517	21.313	37.390	23.110	21.662	-29.051	-20.629	2.972
1600	21.670	38.540	23.890	23.440	-29.313	-20.193	2.758
1700	22.110	39.860	24.784	25.630	-29.607	-19.594	2.519
1800	22.540	41.140	25.657	27.870	-29.879	-18.971	2.303
1900	22.960	42.370	26.507	30.140	-30.149	-18.369	2.113
2000	23.380	43.560	27.330	32.460	-30.397	-17.757	1.940

*Data estimated.

Phase changes:
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2200 K:
$$Cp^\circ = 15.409 + 4.062\times10^{-3}T - 5.987\times10^{5}T^{-2}$$
$$H^\circ - H^\circ_{298} = 15.409\times10^{-3}T + 2.031\times10^{-6}T^{2} + 5.987\times10^{2}T^{-1} - 6.783$$

Formation equations (kcal/mol):

298.15-980 K:
$$\Delta Hf^\circ = -22.913 + 0.325\times10^{-3}T - 1.060\times10^{-6}T^{2} + 122.300T^{-1}$$
$$\Delta Gf^\circ = -22.913 - 0.325\times10^{-3}T\ln T + 1.060\times10^{-6}T^{2} + 61.150T^{-1} + 2.093\times10^{-3}T$$

980-1360 K:
$$\Delta Hf^\circ = -22.494 - 1.856\times10^{-3}T + 0.083\times10^{-6}T^{2} + 209.100T^{-1}$$
$$\Delta Gf^\circ = -22.494 + 1.856\times10^{-3}T\ln T - 0.083\times10^{-6}T^{2} + 104.550T^{-1} - 12.282\times10^{-3}T$$

1360-1410 K:
$$\Delta Hf^\circ = -22.467 - 1.627\times10^{-3}T - 0.353\times10^{-6}T^{2} + 155.700T^{-1}$$
$$\Delta Gf^\circ = -22.467 + 1.627\times10^{-3}T\ln T + 0.353\times10^{-6}T^{2} + 77.850T^{-1} - 11.228\times10^{-3}T$$

1410-1517 K:
$$\Delta Hf^\circ = -22.214 - 2.216\times10^{-3}T - 0.288\times10^{-6}T^{2} + 155.700T^{-1}$$
$$\Delta Gf^\circ = -22.214 + 2.216\times10^{-3}T\ln T + 0.288\times10^{-6}T^{2} + 77.850T^{-1} - 15.586\times10^{-3}T$$

1517-2000 K:
$$\Delta Hf^\circ = -22.969 - 5.037\times10^{-3}T + 0.647\times10^{-6}T^{2} + 155.700T^{-1}$$
$$\Delta Gf^\circ = -22.969 + 5.037\times10^{-3}T\ln T - 0.647\times10^{-6}T^{2} + 77.850T^{-1} - 34.333\times10^{-3}T$$

Source: Data are those estimated by Hack (199).

$Mn_2B(c)$
Dimanganese Boride
[Formation: $2Mn(c,l) + B(\beta) = Mn_2B(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.650	15.890	15.890	0	-21.900	-21.656	15.874
300	13.720	15.980	15.890	.030	-21.899	-21.650	15.772
400	16.200	20.300	16.475	1.530	-22.020	-21.560	11.780
500	17.630	24.080	17.620	3.230	-22.123	-21.423	9.364
600	18.660	27.390	18.973	5.050	-22.262	-21.272	7.748
700	19.500	30.330	20.387	6.960	-22.434	-21.097	6.587
800	20.240	32.980	21.792	8.950	-22.626	-20.890	5.707
900	20.910	35.410	23.177	11.010	-22.835	-20.666	5.018
980	21.422	37.206	24.246	12.700	-23.014	-20.455	4.562
980	21.422	37.206	24.246	12.700	-24.078	-20.455	4.562
1000	21.550	37.640	24.510	13.130	-24.127	-20.387	4.456
1100	22.160	39.720	25.802	15.310	-24.361	-19.994	3.972
1200	22.760	41.680	27.047	17.560	-24.562	-19.606	3.571
1300	23.350	43.520	28.243	19.860	-24.748	-19.184	3.225
1360	23.698	44.580	28.942	21.267	-24.849	-18.909	3.039
1360	23.698	44.580	28.942	21.267	-25.863	-18.909	3.039
1400	23.930	45.270	29.399	22.220	-26.000	-18.706	2.920
1410	23.986	45.441	29.512	22.460	-26.034	-18.635	2.888
1410	23.986	45.441	29.512	22.460	-26.932	-18.635	2.888
1500	24.490	46.940	30.507	24.650	-27.301	-18.091	2.636
1517	24.587	47.217	30.692	25.067	-27.372	-17.968	2.589
1517	24.587	47.217	30.692	25.067	-33.136	-17.968	2.589
1600	25.060	48.540	31.584	27.130	-33.463	-17.127	2.339
1700	25.630	50.090	32.643	29.660	-33.825	-16.111	2.071
1800	26.180	51.560	33.643	32.250	-34.141	-15.025	1.824

*Data estimated.

Phase changes:
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K:
$Cp° = 16.527 + 5.424\times10^{-3}T - 3.995\times10^{5}T^{-2}$
$H°-H°_{298} = 16.527\times10^{-3}T + 2.712\times10^{-6}T^{2} + 3.995\times10^{2}T^{-1} - 6.509$

Formation equations (kcal/mol):

298.15-980 K:
$\Delta Hf° = -22.306 + 0.528\times10^{-3}T - 1.394\times10^{-6}T^{2} + 111.200T^{-1}$
$\Delta Gf° = -22.306 - 0.528\times10^{-3}T\ln T + 1.394\times10^{-6}T^{2} + 55.600T^{-1} + 4.151\times10^{-3}T$

980-1360 K:
$\Delta Hf° = -21.468 - 3.834\times10^{-3}T + 0.892\times10^{-6}T^{2} + 284.800T^{-1}$
$\Delta Gf° = -21.468 + 3.834\times10^{-3}T\ln T - 0.892\times10^{-6}T^{2} + 142.400T^{-1} - 24.598\times10^{-3}T$

1360-1410 K:
$\Delta Hf° = -21.414 - 3.376\times10^{-3}T + 0.020\times10^{-6}T^{2} + 178.000T^{-1}$
$\Delta Gf° = -21.414 + 3.376\times10^{-3}T\ln T - 0.020\times10^{-6}T^{2} + 89.000T^{-1} - 22.491\times10^{-3}T$

1410-1517 K:
$\Delta Hf° = -20.909 - 4.554\times10^{-3}T + 0.150\times10^{-6}T^{2} + 178.000T^{-1}$
$\Delta Gf° = -20.909 + 4.554\times10^{-3}T\ln T - 0.150\times10^{-6}T^{2} + 89.000T^{-1} - 31.207\times10^{-3}T$

1517-1800 K:
$\Delta Hf° = -22.418 - 10.196\times10^{-3}T + 2.020\times10^{-6}T^{2} + 178.000T^{-1}$
$\Delta Gf° = -22.418 + 10.196\times10^{-3}T\ln T - 2.020\times10^{-6}T^{2} + 89.000T^{-1} - 68.701\times10^{-3}T$

Source: Data are those estimated by Hack (199).

$Mn_3B_4(c)$
Trimanganese Tetraboride
[Formation: $3Mn(c,l) + 4B(\beta) = Mn_3B_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	29.030	28.200	28.200	0	-56.700	-56.584	41.476
300	29.210	28.380	28.213	.050	-56.706	-56.583	41.220
400	36.110	37.850	29.450	3.360	-56.620	-56.560	30.903
500	39.890	46.350	31.990	7.180	-56.522	-56.537	24.712
600	42.410	53.840	35.023	11.290	-56.538	-56.556	20.600
700	44.370	60.540	38.183	15.650	-56.596	-56.547	17.655
800	46.010	66.570	41.370	20.160	-56.724	-56.540	15.446
900	47.480	72.080	44.480	24.840	-56.870	-56.510	13.722
980	48.568	76.166	46.905	28.676	-57.011	-56.463	12.592
980	48.568	76.166	46.905	28.676	-58.607	-56.463	12.592
1000	48.840	77.150	47.500	29.650	-58.648	-56.428	12.332
1100	50.110	81.870	50.415	34.600	-58.829	-56.200	11.166
1200	51.340	86.280	53.222	39.670	-58.983	-55.971	10.194
1300	52.530	90.430	55.915	44.870	-59.097	-55.691	9.362
1360	53.232	92.810	57.486	48.041	-59.156	-55.500	8.919
1360	53.232	92.810	57.486	48.041	-60.677	-55.500	8.919
1400	53.700	94.360	58.517	50.180	-60.825	-55.351	8.641
1410	53.816	94.743	58.773	50.718	-60.862	-55.283	8.569
1410	53.816	94.743	58.773	50.718	-62.209	-55.283	8.569
1500	54.860	98.110	61.030	55.620	-62.639	-54.824	7.988
1517	55.054	98.729	61.449	56.554	-62.723	-54.707	7.881
1517	55.054	98.729	61.449	56.554	-71.369	-54.707	7.881
1600	56.000	101.690	63.471	61.150	-71.767	-53.831	7.353
1700	57.120	105.120	65.820	66.810	-72.175	-52.676	6.772
1800	58.240	108.420	68.098	72.580	-72.529	-51.469	6.249
1900	59.350	111.600	70.311	78.450	-72.839	-50.324	5.789
2000	60.440	114.680	72.460	84.440	-73.085	-49.165	5.372

*Data estimated.

Phase changes:
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 39.283 + 10.746\times10^{-3}T - 11.962\times10^{5}T^{-2}$
$H° - H°_{298} = 39.283\times10^{-3}T + 5.373\times10^{-6}T^{2} + 11.962\times10^{2}T^{-1} - 16.202$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = -58.217 + 3.477\times10^{-3}T - 2.516\times10^{-6}T^{2} + 210.000T^{-1}$
$\Delta Gf° = -58.217 - 3.477\times10^{-3}T\ln T + 2.516\times10^{-6}T^{2} + 105.000T^{-1} + 23.358\times10^{-3}T$
980-1360 K: $\Delta Hf° = -56.960 - 3.066\times10^{-3}T + 0.913\times10^{-6}T^{2} + 470.400T^{-1}$
$\Delta Gf° = -56.960 + 3.066\times10^{-3}T\ln T - 0.913\times10^{-6}T^{2} + 235.200T^{-1} - 19.765\times10^{-3}T$
1360-1410 K: $\Delta Hf° = -56.878 - 2.379\times10^{-3}T - 0.395\times10^{-6}T^{2} + 310.200T^{-1}$
$\Delta Gf° = -56.878 + 2.379\times10^{-3}T\ln T + 0.395\times10^{-6}T^{2} + 155.100T^{-1} - 16.604\times10^{-3}T$
1410-1517 K: $\Delta Hf° = -56.122 - 4.146\times10^{-3}T - 0.200\times10^{-6}T^{2} + 310.200T^{-1}$
$\Delta Gf° = -56.122 + 4.146\times10^{-3}T\ln T + 0.200\times10^{-6}T^{2} + 155.100T^{-1} - 29.679\times10^{-3}T$
1517-2000 K: $\Delta Hf° = -58.384 - 12.609\times10^{-3}T + 2.605\times10^{-6}T^{2} + 310.200T^{-1}$
$\Delta Gf° = -58.384 + 12.609\times10^{-3}T\ln T - 2.605\times10^{-6}T^{2} + 155.100T^{-1} - 85.919\times10^{-3}T$

Source: Data are those estimated by Hack (199).

$Mn_3C(c)$
Trimanganese Carbide
[Formation: $3Mn(c,l) + C(c) = Mn_3C(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	22.330	23.600	23.600	0	1.100	1.315	-.964
300	22.396	23.738	23.601	.041	1.101	1.316	-.959
400	24.964	30.597	24.520	2.431	1.291	1.357	-.742
500	26.308	36.322	26.322	5.000	1.449	1.362	-.595
600	27.278	41.208	28.406	7.681	1.527	1.333	-.485
700	28.121	45.477	30.547	10.451	1.527	1.288	-.402
800	28.939	49.285	32.655	13.304	1.467	1.254	-.343
900	29.781	52.742	34.698	16.240	1.366	1.230	-.299
980	30.495	55.307	36.276	18.650	1.272	1.233	-.275
980	30.495	55.307	36.276	18.650	-.324	1.233	-.275
1000	30.673	55.925	36.663	19.262	-.355	1.255	-.274
1100	31.631	58.893	38.550	22.377	-.479	1.458	-.290
1200	32.663	61.689	40.363	25.591	-.551	1.602	-.292
1300	33.774	64.347	42.107	28.912	-.558	1.777	-.299
1310	33.890	64.606	42.278	29.250	-.555	1.795	-.299
1310	38.000	67.182	42.278	32.625	2.820	1.795	-.299
1360	38.000	68.605	43.219	34.525	3.038	1.779	-.286
1360	38.000	68.605	43.219	34.525	1.517	1.779	-.286
1400	38.000	69.707	43.961	36.045	1.570	1.780	-.278
1410	38.000	69.977	44.144	36.425	1.582	1.810	-.281
1410	38.000	69.977	44.144	36.425	.235	1.810	-.281
1500	38.000	72.329	45.766	39.845	.200	1.895	-.276
1517	38.000	72.757	46.066	40.491	.188	1.942	-.280
1517	38.000	72.757	46.066	40.491	-8.458	1.942	-.280
1600	38.000	74.782	47.504	43.645	-8.520	2.533	-.346
1700	38.000	77.085	49.176	47.445	-8.602	3.242	-.417
1800	38.000	79.257	50.788	51.245	-8.689	3.949	-.479

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1310 K, α - β transition point of Mn_3C; ΔH° = 3.375 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1310 K: $C_p^\circ = 23.922 + 7.264\times10^{-3}T - 3.341\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 23.922\times10^{-3}T + 3.632\times10^{-6}T^2 + 3.341\times10^{2}T^{-1} - 8.576$
1310-1800 K: $C_p^\circ = 38.000$
$H^\circ - H^\circ_{298} = 38.000\times10^{-3}T - 17.155$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf^\circ = 0.053 + 3.490\times10^{-3}T - 2.255\times10^{-6}T^2 + 61.600T^{-1}$
$\Delta Gf^\circ = 0.053 - 3.490\times10^{-3}T\ln T + 2.255\times10^{-6}T^2 + 30.800T^{-1} + 23.098\times10^{-3}T$
980-1310 K: $\Delta Hf^\circ = 1.311 - 3.053\times10^{-3}T + 1.174\times10^{-6}T^2 + 322.000T^{-1}$
$\Delta Gf^\circ = 1.311 + 3.053\times10^{-3}T\ln T - 1.174\times10^{-6}T^2 + 161.000T^{-1} - 20.025\times10^{-3}T$
1310-1360 K: $\Delta Hf^\circ = -7.269 + 11.025\times10^{-3}T - 2.458\times10^{-6}T^2 - 12.100T^{-1}$
$\Delta Gf^\circ = -7.269 - 11.025\times10^{-3}T\ln T + 2.458\times10^{-6}T^2 - 6.050T^{-1} + 82.912\times10^{-3}T$
1360-1410 K: $\Delta Hf^\circ = -7.187 + 11.712\times10^{-3}T - 3.766\times10^{-6}T^2 - 172.300T^{-1}$
$\Delta Gf^\circ = -7.187 - 11.712\times10^{-3}T\ln T + 3.766\times10^{-6}T^2 - 86.150T^{-1} + 86.074\times10^{-3}T$
1410-1517 K: $\Delta Hf^\circ = -6.430 + 9.945\times10^{-3}T - 3.571\times10^{-6}T^2 - 172.300T^{-1}$
$\Delta Gf^\circ = -6.430 - 9.945\times10^{-3}T\ln T + 3.571\times10^{-6}T^2 - 86.150T^{-1} + 72.999\times10^{-3}T$
1517-1800 K: $\Delta Hf^\circ = -8.693 + 1.482\times10^{-3}T - 0.766\times10^{-6}T^2 - 172.300T^{-1}$
$\Delta Gf^\circ = -8.693 - 1.482\times10^{-3}T\ln T + 0.766\times10^{-6}T^2 - 86.150T^{-1} + 16.758\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Low-temperature heat capacities and entropy at 298 K from Kelley (247). High-temperature data based on Southard (470).

Mn_7C_3(c)
Heptamanganese Tricarbide
[Formation: 7Mn(c) + 3C(c) = Mn_7C_3(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	56.350	57.100	57.100	0	-26.100	-25.931	19.008
300	56.420	57.450	57.117	.100	-26.096	-25.936	18.894
400	59.410	74.100	59.325	5.910	-25.582	-25.954	14.181
500	61.990	87.640	63.680	11.980	-25.349	-26.069	11.394
600	64.400	99.160	68.660	18.300	-25.354	-26.223	9.552
700	66.740	109.260	73.746	24.860	-25.540	-26.374	8.234
800	69.040	118.330	78.768	31.650	-25.853	-26.487	7.236
900	71.320	126.590	83.634	38.660	-26.254	-26.557	6.449
980	73.120	132.738	87.388	44.443	-26.583	-26.539	5.918
980	73.120	132.738	87.388	44.443	-30.307	-26.539	5.918
1000	73.570	134.220	88.310	45.910	-30.409	-26.484	5.788
1100	75.820	141.340	92.813	53.380	-30.846	-25.982	5.162
1200	78.070	148.030	97.130	61.080	-31.172	-25.605	4.663
1300	80.310	154.370	101.301	68.990	-31.394	-25.155	4.229
1360	81.648	158.020	103.714	73.856	-31.458	-24.791	3.984
1360	81.648	158.020	103.714	73.856	-35.007	-24.791	3.984
1400	82.540	160.400	105.300	77.140	-35.295	-24.500	3.825
1410	82.763	160.988	105.693	77.967	-35.366	-24.356	3.775
1410	82.763	160.988	105.693	77.967	-38.509	-24.356	3.775
1500	84.770	166.170	109.170	85.500	-39.377	-23.467	3.419

*Entropy and heat capacity at 298 K estimated. Data extrapolated above 1100 K.

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 51.532 + 22.214\times10^{-3}T - 1.605\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 51.532\times10^{-3}T + 11.107\times10^{-6}T^{2} + 1.605\times10^{2}T^{-1} - 16.890$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf^\circ = -24.292 + 1.512\times10^{-3}T - 3.140\times10^{-6}T^{2} - 590.200T^{-1}$
$\Delta Gf^\circ = -24.292 - 1.512\times10^{-3}T\ln T + 3.140\times10^{-6}T^{2} - 295.100T^{-1} + 5.501\times10^{-3}T$
980-1360 K: $\Delta Hf^\circ = -21.359 - 13.755\times10^{-3}T + 4.861\times10^{-6}T^{2} + 17.400T^{-1}$
$\Delta Gf^\circ = -21.359 + 13.755\times10^{-3}T\ln T - 4.861\times10^{-6}T^{2} + 8.700T^{-1} - 95.120\times10^{-3}T$
1360-1410 K: $\Delta Hf^\circ = -21.168 - 12.152\times10^{-3}T + 1.809\times10^{-6}T^{2} - 356.400T^{-1}$
$\Delta Gf^\circ = -21.168 + 12.152\times10^{-3}T\ln T - 1.809\times10^{-6}T^{2} - 178.200T^{-1} - 87.744\times10^{-3}T$
1410-1500 K: $\Delta Hf^\circ = -19.402 - 16.275\times10^{-3}T + 2.264\times10^{-6}T^{2} - 356.400T^{-1}$
$\Delta Gf^\circ = -19.402 + 16.275\times10^{-3}T\ln T - 2.264\times10^{-6}T^{2} - 178.200T^{-1} - 118.252\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on McCabe (325). Entropy at 298 K is that estimated by Gokcen (175). High-temperature data based on Bolgar (47). Data extrapolated above 1100 K.

$Mn_{15}C_4(c)$
Manganese Carbide
[Formation: $15Mn(c) + 4C(c) = Mn_{15}C_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	107.070	32.500	32.500	0	-42.000	-15.841	11.612
300	107.190	33.160	32.500	.200	-41.996	-15.677	11.421
400	112.880	64.810	36.785	11.210	-41.742	-6.973	3.810
500	117.780	90.530	45.010	22.760	-41.930	1.779	-.778
600	122.370	112.410	54.460	34.770	-42.558	10.564	-3.848
700	126.810	131.610	64.139	47.230	-43.524	19.437	-6.068
800	131.180	148.830	73.668	60.130	-44.730	28.491	-7.783
900	135.500	164.530	82.897	73.470	-46.088	37.715	-9.158
980	138.932	176.215	90.048	84.443	-47.232	45.259	-10.093
980	138.932	176.215	90.048	84.443	-55.212	45.259	-10.093
1000	139.790	179.030	91.800	87.230	-55.536	47.264	-10.329
1100	144.070	192.550	100.341	101.430	-57.007	57.796	-11.483
1200	148.330	205.270	108.562	116.050	-58.279	68.119	-12.406
1300	152.580	217.310	116.472	131.090	-59.329	78.669	-13.225
1360	155.130	224.249	121.071	140.321	-59.850	85.190	-13.690
1360	155.130	224.249	121.071	140.321	-67.455	85.190	-13.690
1400	156.830	228.770	124.084	146.560	-68.325	89.662	-13.997
1410	157.254	229.888	124.831	148.130	-68.540	90.935	-14.095
1410	157.254	229.888	124.831	148.130	-75.275	90.935	-14.095
1500	161.070	239.740	131.433	162.460	-77.707	101.537	-14.794

*Data at 298 K estimated. Data extrapolated abvoe 1100 K.

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 97.998 + 42.112x10^{-3}T - 3.097x10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 97.998x10^{-3}T + 21.056x10^{-6}T^{2} + 3.097x10^{2}T^{-1} - 32.129$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf^\circ = -38.178 - 0.644x10^{-3}T - 7.613x10^{-6}T^{2} - 880.500T^{-1}$
$\Delta Gf^\circ = -38.178 + 0.644x10^{-3}T\ln T + 7.613x10^{-6}T^{2} - 440.250T^{-1} + 73.933x10^{-3}T$
980-1360 K: $\Delta Hf^\circ = -31.892 - 33.359x10^{-3}T + 9.532x10^{-6}T^{2} + 421.500T^{-1}$
$\Delta Gf^\circ = -31.892 + 33.359x10^{-3}T\ln T - 9.532x10^{-6}T^{2} + 210.750T^{-1} - 141.684x10^{-3}T$
1360-1410 K: $\Delta Hf^\circ = -31.483 - 29.924x10^{-3}T + 2.992x10^{-6}T^{2} - 379.500T^{-1}$
$\Delta Gf^\circ = -31.483 + 29.924x10^{-3}T\ln T - 2.992x10^{-6}T^{2} - 189.750T^{-1} - 125.878x10^{-3}T$
1410-1500 K: $\Delta Hf^\circ = -27.699 - 38.759x10^{-3}T + 3.967x10^{-6}T^{2} - 379.500T^{-1}$
$\Delta Gf^\circ = -27.699 + 38.759x10^{-3}T\ln T - 3.967x10^{-6}T^{2} - 189.750T^{-1} - 191.252x10^{-3}T$

Sources: Data at 298 K estimated. High-temperature data based on Bolgar (47). Data extrapolated above 1100 K.

$Mn_{23}C_6$(c)
Manganese Carbide
[Formation: 23Mn(c) + 6C(c) = $Mn_{23}C_6$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	163.420	186.740	186.740	0	-58.680	-59.443	43.572
300	163.610	187.750	186.750	.300	-58.680	-59.451	43.309
400	172.280	236.050	193.200	17.140	-58.300	-59.769	32.656
500	179.760	275.310	205.830	34.740	-58.656	-60.070	26.256
600	186.770	308.710	220.243	53.080	-59.644	-60.278	21.956
700	193.550	338.020	235.034	72.090	-61.164	-60.362	18.846
800	200.220	364.300	249.575	91.780	-63.042	-60.151	16.432
900	206.810	388.260	263.671	112.130	-65.164	-59.687	14.494
980	212.058	406.093	274.577	128.886	-66.933	-59.043	13.167
980	212.058	406.093	274.577	128.886	-79.169	-59.043	13.167
1000	213.370	410.390	277.250	133.140	-79.672	-58.702	12.829
1100	219.890	431.030	290.294	154.810	-81.961	-56.228	11.171
1200	226.400	450.440	302.840	177.120	-83.947	-54.057	9.845
1300	232.890	468.820	314.912	200.080	-85.585	-51.541	8.665
1360	236.778	479.419	321.936	214.177	-86.397	-49.740	7.993
1360	236.778	479.419	321.936	214.177	-98.058	-49.740	7.993
1400	239.370	486.320	326.534	223.700	-99.405	-48.344	7.547
1410	240.017	488.026	327.674	226.097	-99.738	-47.759	7.403
1410	240.017	488.026	327.674	226.097	-110.065	-47.759	7.403
1500	245.840	503.050	337.743	247.960	-113.835	-43.779	6.379

*Heat capacity at 298 K estimated. Data extrapolated above 1100 K.

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 149.476 + 64.380\times10^{-3}T - 4.668\times10^{5}T^{-2}$
$H°-H°_{298} = 149.476\times10^{-3}T + 32.190\times10^{-6}T^{2} + 4.668\times10^{2}T^{-1} - 48.993$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = -52.775 - 1.306\times10^{-3}T - 11.667\times10^{-6}T^{2} - 1335.200T^{-1}$
$\Delta Gf° = -52.775 + 1.306\times10^{-3}T\ln T + 11.667\times10^{-6}T^{2} - 667.600T^{-1} - 25.772\times10^{-3}T$
980-1360 K: $\Delta Hf° = -43.137 - 51.469\times10^{-3}T + 14.622\times10^{-6}T^{2} + 661.200T^{-1}$
$\Delta Gf° = -43.137 + 51.469\times10^{-3}T\ln T - 14.622\times10^{-6}T^{2} + 330.600T^{-1} - 356.384\times10^{-3}T$
1360-1410 K: $\Delta Hf° = -42.510 - 46.202\times10^{-3}T + 4.594\times10^{-6}T^{2} - 567.000T^{-1}$
$\Delta Gf° = -42.510 + 46.202\times10^{-3}T\ln T - 4.594\times10^{-6}T^{2} - 283.500T^{-1} - 332.148\times10^{-3}T$
1410-1500 K: $\Delta Hf° = -36.708 - 59.749\times10^{-3}T + 6.089\times10^{-6}T^{2} - 567.000T^{-1}$
$\Delta Gf° = -36.708 + 59.749\times10^{-3}T\ln T - 6.089\times10^{-6}T^{2} - 283.500T^{-1} - 432.389\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Dawson (111). Entropy at 298 K based on Moattar (336). Heat capacity at 298 K estimated. High-temperature data based on Bolgar (47). Data extrapolated above 1100 K.

$MnCO_3(c)$
Manganese Carbonate
[Formation: $Mn(c) + C(c) + 1.5O_2(g) = MnCO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	18.050	23.900	23.900	0	-212.417	-194.937	142.891
300	18.140	24.010	23.900	.033	-212.420	-194.828	141.930
400	22.970	30.000	24.683	2.127	-212.287	-188.975	103.250
500	25.150	35.390	26.302	4.544	-211.981	-183.182	80.068
600	26.300	40.080	28.210	7.122	-211.655	-177.449	64.635
700	26.960	44.190	30.207	9.788	-211.362	-171.777	53.630

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 29.333 - 0.494\times10^{-3}T - 9.872\times10^{5}T^{-2}$

$H°-H°_{298} = 29.333\times10^{-3}T - 0.247\times10^{-6}T^{2} + 9.872\times10^{2}T^{-1} - 12.035$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -217.284 + 9.332\times10^{-3}T - 3.475\times10^{-6}T^{2} + 713.700T^{-1}$

$\Delta Gf° = -217.284 - 9.332\times10^{-3}T\ln T + 3.475\times10^{-6}T^{2} + 356.850T^{-1} + 123.074\times10^{-3}T$

Source: Data from Chang (74).

$Mn_{0.9554}Ca_{0.0446}SiO_3$(pyroxmanganite)

Pyroxmanganite
[Formation: 0.9554Mn(c,l) + 0.0446Ca(c,l,g) + Si(c,l)
+ $1.5O_2$(g) = $Mn_{0.9554}Ca_{0.0446}SiO_3$(c)]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	21.029	23.785	23.785	0	-319.668	-301.190	220.776
300	21.097	23.915	23.785	.039	-319.669	-301.075	219.330
400	25.202	30.606	24.671	2.374	-319.557	-294.890	161.118
500	27.511	36.500	26.460	5.020	-319.249	-288.752	126.212
600	28.987	41.654	28.572	7.849	-318.864	-282.690	102.969
700	30.116	46.210	30.773	10.806	-318.445	-276.698	86.388
720	30.302	47.061	31.214	11.410	-318.358	-275.506	83.627
720	30.302	47.061	31.214	11.410	-318.368	-275.506	83.627
800	31.048	50.295	32.962	13.866	-318.011	-270.764	73.968
900	31.729	53.994	35.097	17.007	-317.559	-264.885	64.322
980	31.979	56.710	36.752	19.559	-317.202	-260.209	58.028
980	31.979	56.710	36.752	19.559	-317.711	-260.209	58.028
1000	32.042	57.357	37.158	20.199	-317.627	-259.039	56.612
1100	31.938	60.409	39.134	23.402	-317.230	-253.198	50.305
1112	31.894	60.755	39.366	23.785	-317.186	-252.500	49.625
1112	31.894	60.755	39.366	23.785	-317.277	-252.500	49.625
1200	31.575	63.173	41.025	26.578	-316.970	-247.394	45.056
1300	31.456	65.692	42.827	29.724	-316.673	-241.611	40.618
1350	31.772	66.884	43.697	31.303	-316.531	-238.713	38.644

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
980 K, α - β transition point of Mn; ΔH° = 0.532 kca/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1350 K: $Cp^\circ = 29.627 + 2.756\times10^{-3}T - 8.374\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 29.627\times10^{-3}T + 1.378\times10^{-6}T^2 + 8.374\times10^{2}T^{-1} - 11.764$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -323.940 + 7.546\times10^{-3}T - 1.473\times10^{-6}T^2 + 641.910T^{-1}$
$\Delta Gf^\circ = -323.940 - 7.546\times10^{-3}T\ln T + 1.473\times10^{-6}T^2 + 320.955T^{-1} + 115.244\times10^{-3}T$

720-980 K: $\Delta Hf^\circ = -324.017 + 7.721\times10^{-3}T - 1.579\times10^{-6}T^2 + 639.190T^{-1}$
$\Delta Gf^\circ = -324.017 - 7.721\times10^{-3}T\ln T + 1.579\times10^{-6}T^2 + 319.595T^{-1} + 116.434\times10^{-3}T$

980-1112 K: $\Delta Hf^\circ = -323.617 + 5.638\times10^{-3}T - 0.487\times10^{-6}T^2 + 722.118T^{-1}$
$\Delta Gf^\circ = -323.617 - 5.638\times10^{-3}T\ln T + 0.487\times10^{-6}T^2 + 361.059T^{-1} + 102.701\times10^{-3}T$

1112-1350 K: $\Delta Hf^\circ = -323.628 + 5.321\times10^{-3}T - 0.266\times10^{-6}T^2 + 722.118T^{-1}$
$\Delta Gf^\circ = -323.628 - 5.321\times10^{-3}T\ln T + 0.266\times10^{-6}T^2 + 361.059T^{-1} + 100.733\times10^{-3}T$

Source: Data from Bennington (32).

$MnFe_2O_4(c)$
Manganese Ferrite
[Formation: $Mn(c) + 2Fe(c) + 2O_2(g) = MnFe_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	39.009	39.000	39.000	0	-290.000	-266.237	195.155
300	39.139	39.242	39.002	.072	-289.988	-266.090	193.844
350	42.302	45.520	39.489	2.111	-289.586	-262.138	163.684
400	45.085	51.352	40.612	4.296	-289.088	-258.250	141.099
450	47.807	56.819	42.112	6.618	-288.502	-254.427	123.565
500	50.726	62.004	43.844	9.080	-287.828	-250.676	109.569
550	54.071	66.992	45.723	11.698	-287.047	-246.998	98.147
580	56.369	69.923	46.899	13.354	-286.518	-244.827	92.252
600	51.407	71.742	47.697	14.427	-286.207	-243.395	88.655
650	47.135	75.637	49.702	16.858	-285.714	-239.852	80.644
700	46.575	79.105	51.679	19.198	-285.364	-236.337	73.787
750	46.028	82.299	53.615	21.513	-285.091	-232.849	67.851

*Entropy at 298 K estimated.

Phase change: 580 K, second order transition point of $MnFe_2O_4$; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-580 K: $Cp° = 23.005 + 56.500\times10^{-3}T - 0.748\times10^{5}T^{-2}$

$H°-H°_{298} = 23.005\times10^{-3}T + 28.250\times10^{-6}T^2 + 0.748\times10^{2}T^{-1} - 9.621$

580-750 K: $Cp° = 75.432 - 41.258\times10^{-3}T$

$H°-H°_{298} = 75.432\times10^{-3}T - 20.629\times10^{-6}T^2 - 23.457$

Formation equations (kcal/mol):

298.15-580 K: $\Delta Hf° = -293.558 + 3.349\times10^{-3}T + 13.395\times10^{-6}T^2 + 408.000T^{-1}$

$\Delta Gf° = -293.558 - 3.349\times10^{-3}T\ln T - 13.395\times10^{-6}T^2 + 204.000T^{-1} + 112.413\times10^{-3}T$

580-750 K: $\Delta Hf° = -307.393 + 55.776\times10^{-3}T - 35.484\times10^{-6}T^2 + 333.200T^{-1}$

$\Delta Gf° = -307.393 - 55.776\times10^{-3}T\ln T + 35.484\times10^{-6}T^2 + 166.600T^{-1} + 441.623\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Bulgakova (62). Entropy at 298 K estimated. Other data based on Naito (347).

$Mn_4N(c)$
Tetramanganese Nitride
[Formation: $4Mn(c) + 0.5N_2(g) = Mn_4N(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	29.830	34.160	34.160	0	-30.750	-24.988	18.317
300	29.910	34.350	34.163	.056	-30.749	-24.954	18.178
400	33.440	43.480	35.382	3.239	-30.522	-23.054	12.596
500	35.140	51.150	37.788	6.681	-30.224	-21.212	9.272
600	35.730	57.620	40.570	10.230	-29.999	-19.437	7.080

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 38.201 - 0.500\times10^{-3}T - 7.309\times10^{5}T^{-2}$

$H°-H°_{298} = 38.201\times10^{-3}T - 0.250\times10^{-6}T^{2} + 7.309\times10^{2}T^{-1} - 13.819$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = -35.805 + 12.391\times10^{-3}T - 7.372\times10^{-6}T^{2} + 601.250T^{-1}$

$\Delta Gf° = -35.805 - 12.391\times10^{-3}T\ln T + 7.372\times10^{-6}T^{2} + 300.625T^{-1} + 101.297\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Other data from Garcia (170).

$Mn_5N_2(c)$
Pentamanganese Dinitride
[Formation: $5Mn(c) + N_2(g) = Mn_5N_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	41.999	44.800	44.800	0	-48.800	-37.107	27.199
300	42.070	45.060	44.800	.078	-48.795	-37.034	26.979
400	45.910	57.689	46.496	4.477	-48.353	-33.181	18.129
500	49.750	68.346	49.826	9.260	-47.763	-29.443	12.869
600	53.590	77.756	53.711	14.427	-47.019	-25.852	9.416
700	57.430	86.305	57.765	19.978	-46.105	-22.409	6.996
800	61.270	94.224	61.833	25.913	-45.003	-19.104	5.219

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 30.550 + 38.400x10^{-3}T$

$H°- H°_{298} = 30.550x10^{-3}T + 19.200x10^{-6}T^2 - 10.815$

Formation equations (kcal/mol):

298.15-800 K: $ΔHf° = -47.923 - 4.157x10^{-3}T + 10.076x10^{-6}T^2 - 159.100T^{-1}$

$ΔGf° = -47.923 + 4.157x10^{-3}TlnT - 10.076x10^{-6}T^2 - 79.550T^{-1} + 16.492x10^{-3}T$

Source: Data from Barin (23).

$MnO(g)$
Manganese Monoxide (ideal gas)
[Formation: $Mn(c,l) + 0.5O_2(g) = MnO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.580	56.677	56.677	0	31.000	23.688	-17.364
300	7.580	56.724	56.677	.014	30.996	23.643	-17.223
400	7.950	58.957	56.979	.791	30.766	21.225	-11.596
500	8.230	60.762	57.560	1.601	30.512	18.871	-8.249
600	8.410	62.280	58.225	2.433	30.224	16.568	-6.035
700	8.540	63.587	58.900	3.281	29.901	14.313	-4.469
800	8.640	64.734	59.558	4.141	29.544	12.109	-3.308
900	8.700	65.755	60.191	5.008	29.154	9.953	-2.417
980	8.748	66.498	60.676	5.706	28.822	8.263	-1.843
980	8.748	66.498	60.676	5.706	28.290	8.263	-1.843
1000	8.760	66.675	60.794	5.881	28.202	7.852	-1.716
1100	8.800	67.512	61.367	6.759	27.755	5.847	-1.162
1200	8.830	68.279	61.912	7.640	27.296	3.867	-.704
1300	8.860	68.987	62.429	8.525	26.828	1.932	-.325
1360	8.872	69.387	62.727	9.057	26.540	.799	-.128
1360	8.872	69.387	62.727	9.057	26.033	.799	-.128
1400	8.880	69.644	62.921	9.412	25.800	.058	-.009
1410	8.882	69.707	62.969	9.501	25.742	-.116	.018
1410	8.882	69.707	62.969	9.501	25.293	-.116	.018
1500	8.900	70.258	63.391	10.301	24.720	-1.727	.252
1517	8.903	70.358	63.468	10.452	24.611	-2.017	.291
1517	8.903	70.358	63.468	10.452	21.729	-2.017	.291
1600	8.920	70.833	63.838	11.192	21.191	-3.295	.450
1700	8.930	71.374	64.266	12.084	20.542	-4.800	.617
1800	8.940	71.885	64.675	12.978	19.892	-6.269	.761
1900	8.960	72.369	65.067	13.873	19.240	-7.714	.887
2000	8.970	72.828	65.443	14.770	18.587	-9.103	.995

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.465 + 0.318\times10^{-3}T - 0.871\times10^{5}T^{-2}$
$H°-H°_{298} = 8.465\times10^{-3}T + 0.159\times10^{-6}T^{2} + 0.871\times10^{2}T^{-1} - 2.830$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = 31.291 - 0.788\times10^{-3}T - 1.799\times10^{-6}T^{2} + 31.100T^{-1}$
$\Delta Gf° = 31.291 + 0.788\times10^{-3}T\ln T + 1.799\times10^{-6}T^{2} + 15.550T^{-1} - 30.700\times10^{-3}T$
980-1360 K: $\Delta Hf° = 31.710 - 2.969\times10^{-3}T - 0.656\times10^{-6}T^{2} + 117.900T^{-1}$
$\Delta Gf° = 31.710 + 2.969\times10^{-3}T\ln T + 0.656\times10^{-6}T^{2} + 58.950T^{-1} - 45.075\times10^{-3}T$
1360-1410 K: $\Delta Hf° = 31.737 - 2.740\times10^{-3}T - 1.092\times10^{-6}T^{2} + 64.500T^{-1}$
$\Delta Gf° = 31.737 + 2.740\times10^{-3}T\ln T + 1.092\times10^{-6}T^{2} + 32.250T^{-1} - 44.021\times10^{-3}T$
1410-1517 K: $\Delta Hf° = 31.989 - 3.329\times10^{-3}T - 1.027\times10^{-6}T^{2} + 64.500T^{-1}$
$\Delta Gf° = 31.989 + 3.329\times10^{-3}T\ln T + 1.027\times10^{-6}T^{2} + 32.250T^{-1} - 48.379\times10^{-3}T$
1517-2000 K: $\Delta Hf° = 31.235 - 6.150\times10^{-3}T - 0.092\times10^{-6}T^{2} + 64.500T^{-1}$
$\Delta Gf° = 31.235 + 6.150\times10^{-3}T\ln T + 0.092\times10^{-6}T^{2} + 32.250T^{-1} - 67.126\times10^{-3}T$

Source: Data from Pedley (396).

MnP(c)
Manganese Phosphide
[Formation: $Mn(c) + P(c,l,1/4P_4(g)) = MnP(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.200	15.600	15.600	0	-27.000	-26.442	19.383
300	11.234	15.669	15.600	.021	-27.002	-26.439	19.261
317.3	11.440	16.305	15.620	.217	-27.014	-26.405	18.187
317.3	11.440	16.305	15.620	.217	-27.171	-26.405	18.187
400	12.425	19.087	16.059	1.211	-27.240	-26.198	14.314
500	12.987	21.927	16.957	2.485	-27.293	-25.929	11.333
550	13.142	23.174	17.465	3.140	-27.319	-25.806	10.254
550	13.142	23.174	17.465	3.140	-30.227	-25.806	10.254
600	13.296	24.324	17.989	3.801	-30.175	-25.406	9.254
700	13.485	26.389	19.045	5.141	-30.089	-24.621	7.687
800	13.611	28.198	20.078	6.496	-30.030	-23.845	6.514
900	13.699	29.807	21.073	7.861	-29.997	-23.076	5.604
980	13.751	30.976	21.833	8.960	-29.986	-22.458	5.008
980	13.751	30.976	21.833	8.960	-30.518	-22.458	5.008
1000	13.764	31.254	22.019	9.235	-30.520	-22.296	4.873
1100	13.814	32.568	22.919	10.614	-30.533	-21.465	4.265
1200	13.854	33.772	23.774	11.997	-30.555	-20.649	3.761
1300	13.887	34.882	24.587	13.384	-30.584	-19.824	3.333

*Heat capacity at 298 K estimated.

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp° = 13.918 + 0.090\times10^{-3}T - 2.439\times10^{5}T^{-2}$
$H°-H°_{298} = 13.918\times10^{-3}T + 0.045\times10^{-6}T^2 + 2.439\times10^{2}T^{-1} - 4.972$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -28.611 + 4.481\times10^{-3}T - 4.847\times10^{-6}T^2 + 210.500T^{-1}$
$\Delta Gf° = -28.611 - 4.481\times10^{-3}T\ln T + 4.847\times10^{-6}T^2 + 105.250T^{-1} + 30.176\times10^{-3}T$
317.3-550 K: $\Delta Hf° = -28.298 + 1.988\times10^{-3}T - 1.662\times10^{-6}T^2 + 210.500T^{-1}$
$\Delta Gf° = -28.298 - 1.988\times10^{-3}T\ln T + 1.662\times10^{-6}T^2 + 105.250T^{-1} + 15.839\times10^{-3}T$
550-980 K: $\Delta Hf° = -31.758 + 3.326\times10^{-3}T - 1.666\times10^{-6}T^2 + 110.200T^{-1}$
$\Delta Gf° = -31.758 - 3.326\times10^{-3}T\ln T + 1.666\times10^{-6}T^2 + 55.100T^{-1} + 30.737\times10^{-3}T$
980-1300 K: $\Delta Hf° = -31.339 + 1.145\times10^{-3}T - 0.523\times10^{-6}T^2 + 197.000T^{-1}$
$\Delta Gf° = -31.339 - 1.145\times10^{-3}T\ln T + 0.523\times10^{-6}T^2 + 98.500T^{-1} + 16.363\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Baratashvili (21). Heat capacity at 298 K estimated. High-temperature data based on Makharadze (322).

$Mn_2P(c)$
Dimanganese Phosphide
[Formation: $2Mn(c) + P(c,l,1/4P_4(g)) = Mn_2P(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	17.577	21.752	21.752	0	-40.900	-39.896	29.244
300	17.608	21.860	21.752	.033	-40.902	-39.890	29.059
317.3	17.842	22.854	21.783	.340	-40.913	-39.830	27.434
317.3	17.842	22.854	21.783	.340	-41.070	-39.830	27.434
400	18.958	27.130	22.462	1.867	-41.148	-39.500	21.581
500	19.902	31.465	23.841	3.812	-41.228	-39.073	17.079
550	20.293	33.382	24.623	4.818	-41.269	-38.872	15.446
550	20.293	33.382	24.623	4.818	-44.177	-38.872	15.446
600	20.684	35.165	25.428	5.842	-44.138	-38.391	13.984
700	21.379	38.406	27.055	7.946	-44.070	-37.445	11.691
800	22.022	41.303	28.658	10.116	-44.014	-36.505	9.973
900	22.624	43.932	30.211	12.349	-43.963	-35.571	8.638
980	23.082	45.879	31.412	14.177	-43.923	-34.820	7.765
980	23.082	45.879	31.412	14.177	-44.987	-34.820	7.765
1000	23.196	46.346	31.706	14.640	-44.981	-34.619	7.566
1100	23.740	48.583	33.140	16.987	-44.931	-33.569	6.669
1200	24.262	50.672	34.516	19.387	-44.852	-32.558	5.930
1300	24.761	52.631	35.832	21.839	-44.742	-31.537	5.302

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp° = 17.880 + 5.458\times10^{-3}T - 1.716\times10^{5}T^{-2}$
$H°-H°_{298} = 17.880\times10^{-3}T + 2.729\times10^{-6}T^{2} + 1.716\times10^{2}T^{-1} - 6.149$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -41.744 + 2.805\times10^{-3}T - 3.870\times10^{-6}T^{2} + 104.800T^{-1}$
$\Delta Gf° = -41.744 - 2.805\times10^{-3}T\ln T + 3.870\times10^{-6}T^{2} + 52.400T^{-1} + 20.437\times10^{-3}T$
317.3-550 K: $\Delta Hf° = -41.430 + 0.312\times10^{-3}T - 0.685\times10^{-6}T^{2} + 104.800T^{-1}$
$\Delta Gf° = -41.430 - 0.312\times10^{-3}T\ln T + 0.685\times10^{-6}T^{2} + 52.400T^{-1} + 6.100\times10^{-3}T$
550-980 K: $\Delta Hf° = -44.891 + 1.650\times10^{-3}T - 0.689\times10^{-6}T^{2} + 4.500T^{-1}$
$\Delta Gf° = -44.891 - 1.650\times10^{-3}T\ln T + 0.689\times10^{-6}T^{2} + 2.250T^{-1} + 20.998\times10^{-3}T$
980-1300 K: $\Delta Hf° = -44.053 - 2.712\times10^{-3}T + 1.597\times10^{-6}T^{2} + 178.100T^{-1}$
$\Delta Gf° = -44.053 + 2.712\times10^{-3}T\ln T - 1.597\times10^{-6}T^{2} + 89.050T^{-1} - 7.751\times10^{-3}T$

Source: Data from Grandjean (181).

$Mn_3P(c)$
Trimanganese Phosphide
[Formation: $3Mn(c) + P(c,l,1/4P_4(g)) = Mn_3P(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	26.320	21.400	21.400	0	-44.000	-40.610	29.768
300	26.400	21.560	21.400	.050	-43.997	-40.588	29.568
317.3	26.910	23.054	21.444	.511	-43.963	-40.391	27.820
317.3	26.910	23.054	21.444	.511	-44.120	-40.391	27.820
400	29.350	29.620	22.470	2.860	-43.919	-39.443	21.550
500	30.720	36.340	24.600	5.870	-43.632	-38.354	16.765
550	31.100	39.287	25.805	7.415	-43.499	-37.852	15.041
550	31.100	39.287	25.805	7.415	-46.407	-37.852	15.041
600	31.480	42.010	27.043	8.980	-46.204	-37.082	13.507
700	31.940	46.900	29.543	12.150	-45.852	-35.603	11.116
800	32.250	51.190	31.990	15.360	-45.574	-34.167	9.334
900	32.470	55.000	34.333	18.600	-45.366	-32.751	7.953
980	32.598	57.771	36.131	21.208	-45.246	-31.620	7.051
980	32.598	57.771	36.131	21.208	-46.842	-31.620	7.051
1000	32.630	58.430	36.570	21.860	-46.827	-31.319	6.845
1100	32.750	61.540	38.695	25.130	-46.759	-29.740	5.909
1200	32.850	64.400	40.725	28.410	-46.716	-28.228	5.141
1300	32.930	67.030	42.645	31.700	-46.694	-26.688	4.487

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.
980 K, α – β transition point of Mn; ΔH° = 0.532 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 33.030 + 0.200\times10^{-3}T - 6.020\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 33.030\times10^{-3}T + 0.100\times10^{-6}T^2 + 6.020\times10^{2}T^{-1} - 11.876$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf^\circ = -48.626 + 12.317\times10^{-3}T - 8.206\times10^{-6}T^2 + 501.800T^{-1}$
$\Delta Gf^\circ = -48.626 - 12.317\times10^{-3}T\ln T + 8.206\times10^{-6}T^2 + 250.900T^{-1} + 91.794\times10^{-3}T$
317.3-550 K: $\Delta Hf^\circ = -48.313 + 9.824\times10^{-3}T - 5.021\times10^{-6}T^2 + 501.800T^{-1}$
$\Delta Gf^\circ = -48.313 - 9.824\times10^{-3}T\ln T + 5.021\times10^{-6}T^2 + 250.900T^{-1} + 77.457\times10^{-3}T$
550-980 K: $\Delta Hf^\circ = -51.773 + 11.162\times10^{-3}T - 5.025\times10^{-6}T^2 + 401.500T^{-1}$
$\Delta Gf^\circ = -51.773 - 11.162\times10^{-3}T\ln T + 5.025\times10^{-6}T^2 + 200.750T^{-1} + 92.355\times10^{-3}T$
980-1300 K: $\Delta Hf^\circ = -50.516 + 4.619\times10^{-3}T - 1.596\times10^{-6}T^2 + 661.900T^{-1}$
$\Delta Gf^\circ = -50.516 - 4.619\times10^{-3}T\ln T + 1.596\times10^{-6}T^2 + 330.950T^{-1} + 49.232\times10^{-3}T$

Source: Data based on Baratashvili (22).

$MnSO_4(c)$
Manganese Sulfate
[Reaction: $Mn(c) + 0.5S_2(g) + 2O_2(g) = MnSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	24.020	26.790	26.790	0	-270.055	-238.414	174.760
300	24.110	26.939	26.790	.045	-270.055	-238.217	173.539
400	28.019	34.470	27.793	2.671	-269.900	-227.623	124.366
500	30.643	41.018	29.796	5.611	-269.534	-217.089	94.888
600	32.674	46.791	32.158	8.780	-269.040	-206.646	75.270
700	34.313	51.956	34.623	12.133	-268.456	-196.295	61.285
800	35.642	56.627	37.086	15.633	-267.806	-186.032	50.821
900	36.702	60.889	39.498	19.252	-267.104	-175.853	42.703
980	37.350	64.044	41.374	22.216	-266.516	-167.764	37.413
980	37.350	64.044	41.374	22.216	-267.048	-167.764	37.413
1000	37.512	64.800	41.835	22.965	-266.901	-165.743	36.223
1100	38.085	68.404	44.089	26.747	-266.150	-155.653	30.925

Phase change: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp^\circ = 28.112 + 10.278\times10^{-3}T - 6.361\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 28.112\times10^{-3}T + 5.139\times10^{-6}T^{2} + 6.361\times10^{2}T^{-1} - 10.972$

Reaction equations (kcal/mol):

298.15-980 K: $\Delta Hr^\circ = -273.006 + 3.842\times10^{-3}T + 2.266\times10^{-6}T^{2} + 478.150T^{-1}$

$\Delta Gr^\circ = -273.006 - 3.842\times10^{-3}T\ln T - 2.266\times10^{-6}T^{2} + 239.075T^{-1} + 135.899\times10^{-3}T$

980-1100 K: $\Delta Hr^\circ = -272.587 + 1.661\times10^{-3}T + 3.409\times10^{-6}T^{2} + 564.950T^{-1}$

$\Delta Gr^\circ = -272.587 - 1.661\times10^{-3}T\ln T - 3.409\times10^{-6}T^{2} + 282.475T^{-1} + 121.525\times10^{-3}T$

Source: Data from DeKock (112).

$MnSO_4 \cdot H_2O(\alpha)$
α-Manganese Sulfate Monohydrate
[Reaction: $Mn(c) + 0.5S_2(g) + 2.5O_2(g) + H_2(g) = MnSO_4 \cdot H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	33.000	35.000	35.000	0	-344.455	-298.652	218.915
300	33.167	35.205	35.002	.061	-344.458	-298.368	217.358
350	37.667	40.655	35.421	1.832	-344.432	-290.687	181.511
400	42.168	45.979	36.409	3.828	-344.212	-283.021	154.634
450	46.669	51.205	37.763	6.049	-343.794	-275.393	133.747
500	51.169	56.355	39.365	8.495	-343.183	-267.823	117.064
550	55.670	61.443	41.141	11.166	-342.374	-260.326	103.443

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 6.119 + 90.094 \times 10^{-3}T + 0.018 \times 10^{5}T^{-2}$

$H° - H°_{298} = 6.119 \times 10^{-3}T + 45.047 \times 10^{-6}T^{2} - 0.018 \times 10^{2}T^{-1} - 5.823$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -339.174 - 28.222 \times 10^{-3}T + 41.503 \times 10^{-6}T^{2} - 165.850T^{-1}$

$\Delta Gr° = -339.174 + 28.222 \times 10^{-3}T\ln T - 41.503 \times 10^{-6}T^{2} - 82.925T^{-1} - 11.578 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$MnSO_4 \cdot 4H_2O(c)$
Manganese Sulfate Tetrahydrate
[Reaction: $Mn(c) + 0.5S_2(g) + 4O_2(g) + 4H_2(g) = MnSO_4 \cdot 4H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	61.000	65.000	65.000	0	-555.155	-468.468	343.392
300	61.266	65.378	65.001	.113	-555.165	-467.929	340.882
350	68.467	75.363	65.774	3.356	-555.234	-453.381	283.100
400	75.668	84.976	67.576	6.960	-554.985	-438.843	239.770
450	82.869	94.304	70.031	10.923	-554.418	-424.354	206.092
500	90.069	103.408	72.914	15.247	-553.529	-409.947	179.185
550	97.270	112.330	76.094	19.930	-552.320	-395.646	157.213

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp^\circ = 18.164 + 143.840\times10^{-3}T - 0.044\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.164\times10^{-3}T + 71.920\times10^{-6}T^{2} + 0.044\times10^{2}T^{-1} - 11.824$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr^\circ = -546.626 - 46.389\times10^{-3}T + 66.365\times10^{-6}T^{2} - 177.950T^{-1}$

$\Delta Gr^\circ = -546.626 + 46.389\times10^{-3}T\ln T - 66.365\times10^{-6}T^{2} - 88.975T^{-1} + 18.625\times10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$MnSO_4 \cdot 5H_2O(c)$
Manganese Sulfate Pentahydrate
[Reaction: $Mn(c) + 0.5S_2(g) + 4.5O_2(g) + 5H_2(g) = MnSO_4 \cdot 5H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	78.000	75.000	75.000	0	-625.655	-525.339	385.079
300	78.333	75.484	75.001	.145	-625.652	-524.716	382.251
350	87.332	88.234	75.988	4.286	-625.346	-507.913	317.151
400	96.332	100.484	78.289	8.878	-624.635	-491.180	268.365
450	105.331	112.349	81.418	13.919	-623.521	-474.559	230.474
500	114.331	123.913	85.091	19.411	-621.998	-458.085	200.226
550	123.330	135.232	89.137	25.352	-620.068	-441.786	175.547

*Entropy at 298 K and data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 24.166 + 180.282 \times 10^{-3}T + 0.074 \times 10^{5}T^{-2}$

$H° - H°_{298} = 24.166 \times 10^{-3}T + 90.141 \times 10^{-6}T^{2} - 0.074 \times 10^{2}T^{-1} - 15.193$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -617.413 - 50.459 \times 10^{-3}T + 83.915 \times 10^{-6}T^{2} - 195.850T^{-1}$

$\Delta Gr° = -617.413 + 50.459 \times 10^{-3}T\ln T - 83.915 \times 10^{-6}T^{2} - 97.925T^{-1} + 47.447 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated entropy at 298 K and data above 298 K.

$MnSO_4 \cdot 7H_2O(c)$
Manganese Sulfate Heptahydrate
[Reaction: $Mn(c) + 0.5S_2(g) + 5.5O_2(g) + 7H_2(g) = MnSO_4 \cdot 7H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	91.000	94.000	94.000	0	-765.755	-637.885	467.576
300	91.444	94.564	94.001	.169	-765.768	-637.091	464.114
350	103.443	109.562	95.159	5.041	-765.775	-615.637	384.416
400	115.442	124.158	97.875	10.513	-765.238	-594.218	324.662
450	127.442	138.448	101.592	16.585	-764.154	-572.899	278.234
500	139.441	152.496	105.982	23.257	-762.518	-551.730	241.158
550	151.440	166.349	110.842	30.529	-760.331	-530.754	210.900

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 19.525 + 239.840 \times 10^{-3}T - 0.029 \times 10^{5}T^{-2}$

$H° - H°_{298} = 19.525 \times 10^{-3}T + 119.920 \times 10^{-6}T^{2} + 0.029 \times 10^{2}T^{-1} - 16.491$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -752.646 - 75.242 \times 10^{-3}T + 112.354 \times 10^{-6}T^{2} - 197.750T^{-1}$

$\Delta Gr° = -752.646 + 75.242 \times 10^{-3}T\ln T - 112.354 \times 10^{-6}T^{2} - 98.875T^{-1} - 9.174 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

MnSe(c)
Manganese Selenide
[Reaction: Mn(c,l) + $0.5Se_2(g)$ = MnSe(c)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	12.200	21.700	21.700	0	-57.650	-53.163	38.969
300	12.200	21.780	21.707	.022	-57.649	-53.137	38.710
400	12.360	25.310	22.182	1.251	-57.569	-51.646	28.217
500	12.530	28.080	23.090	2.495	-57.528	-50.165	21.927
600	12.690	30.380	24.120	3.756	-57.514	-48.697	17.738
700	12.850	32.350	25.161	5.032	-57.525	-47.231	14.746
800	13.010	34.080	26.174	6.325	-57.554	-45.762	12.501
900	13.170	35.620	27.138	7.634	-57.597	-44.286	10.754
980	13.298	36.741	27.871	8.693	-57.638	-43.093	9.610
980	13.298	36.741	27.871	8.693	-58.170	-43.093	9.610
1000	13.330	37.010	28.051	8.959	-58.184	-42.789	9.351
1100	13.490	38.290	28.926	10.300	-58.245	-41.238	8.193
1200	13.650	39.470	29.756	11.657	-58.298	-39.698	7.230
1300	13.810	40.570	30.547	13.030	-58.342	-38.147	6.413
1360	13.906	41.196	31.003	13.862	-58.364	-37.208	5.979
1360	13.906	41.196	31.003	13.862	-58.871	-37.208	5.979
1400	13.970	41.600	31.300	14.420	-58.923	-36.572	5.709
1410	13.986	41.699	31.373	14.560	-58.935	-36.402	5.642
1410	13.986	41.699	31.373	14.560	-59.384	-36.402	5.642
1500	14.130	42.570	32.020	15.825	-59.537	-34.937	5.090
1517	14.159	42.729	32.139	16.065	-59.566	-34.649	4.992
1517	14.159	42.729	32.139	16.065	-62.448	-34.649	4.992
1600	14.300	43.490	32.711	17.247	-62.580	-33.124	4.524

*Data except enthalpy of formation at 298 K estimated.

Phase changes:
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K:
$Cp° = 11.720 + 1.610\times10^{-3}T$
$H° - H°_{298} = 11.720\times10^{-3}T + 0.805\times10^{-6}T^2 - 3.566$

Reaction equations (kcal/mol):

298.15-980 K:
$\Delta Hr° = -57.595 + 0.750\times10^{-3}T - 0.742\times10^{-6}T^2 - 63.350T^{-1}$
$\Delta Gr° = -57.595 - 0.750\times10^{-3}T\ln T + 0.742\times10^{-6}T^2 - 31.675T^{-1} + 19.274\times10^{-3}T$

980-1360 K:
$\Delta Hr° = -57.176 - 1.431\times10^{-3}T + 0.400\times10^{-6}T^2 + 23.450T^{-1}$
$\Delta Gr° = -57.176 + 1.431\times10^{-3}T\ln T - 0.400\times10^{-6}T^2 + 11.725T^{-1} + 4.900\times10^{-3}T$

1360-1410 K:
$\Delta Hr° = -57.149 - 1.202\times10^{-3}T - 0.035\times10^{-6}T^2 - 29.950T^{-1}$
$\Delta Gr° = -57.149 + 1.202\times10^{-3}T\ln T + 0.035\times10^{-6}T^2 - 14.975T^{-1} + 5.953\times10^{-3}T$

1410-1517 K:
$\Delta Hr° = -56.897 - 1.791\times10^{-3}T + 0.030\times10^{-6}T^2 - 29.950T^{-1}$
$\Delta Gr° = -56.897 + 1.791\times10^{-3}T\ln T - 0.030\times10^{-6}T^2 - 14.975T^{-1} + 1.595\times10^{-3}T$

1517-1600 K:
$\Delta Hr° = -57.651 - 4.612\times10^{-3}T + 0.965\times10^{-6}T^2 - 29.950T^{-1}$
$\Delta Gr° = -57.651 + 4.612\times10^{-3}T\ln T - 0.965\times10^{-6}T^2 - 14.975T^{-1} - 17.152\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Mills (332), Smoes (467), and Lukashenko (311). Other data are those estimated by Mills (332).

MnSi(c,l)
Manganese Silicide
[Formation: Mn(c,l) + Si(c,l) = MnSi(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.980	11.100	11.100	0	-19.000	-18.687	13.698
300	11.000	11.170	11.103	.020	-19.001	-18.686	13.613
400	12.050	14.490	11.540	1.180	-19.000	-18.580	10.152
500	12.700	17.260	12.420	2.420	-19.004	-18.474	8.075
600	13.200	19.620	13.437	3.710	-19.028	-18.374	6.693
700	13.610	21.680	14.451	5.060	-19.051	-18.253	5.699
800	13.990	23.530	15.480	6.440	-19.094	-18.142	4.956
900	14.350	25.200	16.478	7.850	-19.154	-18.029	4.378
980	14.622	26.424	17.223	9.017	-19.189	-17.898	3.991
980	14.622	26.424	17.223	9.017	-19.721	-17.898	3.991
1000	14.690	26.720	17.410	9.310	-19.734	-17.864	3.904
1100	15.020	28.140	18.331	10.790	-19.796	-17.684	3.513
1200	15.350	29.460	19.202	12.310	-19.836	-17.496	3.186
1300	15.670	30.700	20.038	13.860	-19.862	-17.301	2.909
1360	15.862	31.418	20.534	14.803	-19.874	-17.182	2.761
1360	15.862	31.418	20.534	14.803	-20.381	-17.182	2.761
1400	15.990	31.880	20.851	15.440	-20.421	-17.089	2.668
1410	16.021	31.994	20.930	15.600	-20.431	-17.056	2.644
1410	16.021	31.994	20.930	15.600	-20.880	-17.056	2.644
1500	16.300	32.990	21.617	17.060	-20.998	-16.813	2.450
1517	16.353	33.174	21.745	17.338	-21.021	-16.756	2.414
1517	16.353	33.174	21.745	17.338	-23.903	-16.756	2.414
1548	16.450	33.510	21.984	17.840	-23.948	-16.620	2.346
1548	18.800	42.680	21.984	32.040	-9.748	-16.620	2.346
1600	18.800	43.300	22.662	33.020	-9.688	-16.840	2.300
1687	18.800	44.296	23.753	34.656	-9.595	-17.205	2.229
1687	18.800	44.296	23.753	34.656	-21.677	-17.205	2.229
1700	18.800	44.440	23.911	34.900	-21.655	-17.167	2.207
1800	18.800	45.510	25.077	36.780	-21.485	-16.895	2.051
1900	18.800	46.530	26.183	38.660	-21.315	-16.660	1.916
2000	18.800	47.490	27.220	40.540	-21.145	-16.405	1.793

Phase changes:
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.
1548 K, melting point of MnSi; ΔH° = 14.200 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1548 K: $Cp° = 11.787 + 3.054\times10^{-3}T - 1.532\times10^{5}T^{-2}$
$H°-H°_{298} = 11.787\times10^{-3}T + 1.527\times10^{-6}T^{2} + 1.532\times10^{2}T^{-1} - 4.164$
1548-2000 K: $Cp° = 18.800$
$H°-H°_{298} = 18.800\times10^{-3}T + 2.938$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = -19.164 + 0.470\times10^{-3}T - 0.531\times10^{-6}T^{2} + 21.300T^{-1}$
$\Delta Gf° = -19.164 - 0.470\times10^{-3}T\ln T + 0.531\times10^{-6}T^{2} + 10.650T^{-1} + 4.001\times10^{-3}T$
980-1360 K: $\Delta Hf° = -18.745 - 1.711\times10^{-3}T + 0.612\times10^{-6}T^{2} + 108.100T^{-1}$
$\Delta Gf° = -18.745 + 1.711\times10^{-3}T\ln T - 0.612\times10^{-6}T^{2} + 54.050T^{-1} - 10.373\times10^{-3}T$
1360-1410 K: $\Delta Hf° = -18.718 - 1.482\times10^{-3}T + 0.176\times10^{-6}T^{2} + 54.700T^{-1}$
$\Delta Gf° = -18.718 + 1.482\times10^{-3}T\ln T - 0.176\times10^{-6}T^{2} + 27.350T^{-1} - 9.320\times10^{-3}T$
1410-1517 K: $\Delta Hf° = -18.466 - 2.071\times10^{-3}T + 0.241\times10^{-6}T^{2} + 54.700T^{-1}$
$\Delta Gf° = -18.466 + 2.071\times10^{-3}T\ln T - 0.241\times10^{-6}T^{2} + 27.350T^{-1} - 13.678\times10^{-3}T$
1517-1548 K: $\Delta Hf° = -19.220 - 4.892\times10^{-3}T + 1.176\times10^{-6}T^{2} + 54.700T^{-1}$
$\Delta Gf° = -19.220 + 4.892\times10^{-3}T\ln T - 1.176\times10^{-6}T^{2} + 27.350T^{-1} - 32.425\times10^{-3}T$
1548-1687 K: $\Delta Hf° = -12.118 + 2.121\times10^{-3}T - 0.351\times10^{-6}T^{2} - 98.500T^{-1}$
$\Delta Gf° = -12.118 - 2.121\times10^{-3}T\ln T + 0.351\times10^{-6}T^{2} - 49.250T^{-1} + 12.164\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -24.547 + 1.700\times10^{-3}T$
$\Delta Gf° = -24.547 - 1.700\times10^{-3}T\ln T + 16.978\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Eremenko (140). Other data from Chart (77).

$MnSi_{1.7}(c)$
Manganese Silicide
[Formation: $Mn(c) + 1.7Si(c) = MnSi_{1.7}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	14.020	13.400	13.400	0	-22.000	-21.434	15.711
300	14.070	13.490	13.400	.030	-21.997	-21.427	15.609
400	15.700	17.790	13.965	1.530	-22.011	-21.237	11.603
500	16.510	21.390	15.110	3.140	-22.027	-21.042	9.198
600	17.000	24.440	16.407	4.820	-22.062	-20.839	7.591
700	17.340	27.090	17.761	6.530	-22.139	-20.644	6.445
800	17.600	29.420	19.070	8.280	-22.235	-20.417	5.578
900	17.820	31.510	20.343	10.050	-22.369	-20.188	4.902
980	17.964	33.037	21.322	11.480	-22.491	-19.976	4.455
980	17.964	33.037	21.322	11.480	-23.023	-19.976	4.455
1000	18.000	33.400	21.560	11.840	-23.059	-19.917	4.353
1100	18.160	35.120	22.711	13.650	-23.237	-19.593	3.893
1200	18.320	36.710	23.810	15.480	-23.417	-19.260	3.508
1300	18.460	38.180	24.857	17.320	-23.608	-18.905	3.178
1360	18.538	39.012	25.462	18.427	-23.731	-18.667	3.000
1360	18.538	39.012	25.462	18.427	-24.238	-18.667	3.000
1400	18.590	39.550	25.857	19.170	-24.357	-18.504	2.889

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 17.208 + 1.104 \times 10^{-3}T - 3.126 \times 10^{5}T^{-2}$
$H° - H°_{298} = 17.208 \times 10^{-3}T + 0.552 \times 10^{-6}T^{2} + 3.126 \times 10^{2}T^{-1} - 6.228$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = -22.790 + 1.916 \times 10^{-3}T - 1.752 \times 10^{-6}T^{2} + 111.750T^{-1}$
$\Delta Gf° = -22.790 - 1.916 \times 10^{-3}T\ln T + 1.752 \times 10^{-6}T^{2} + 55.875T^{-1} + 14.315 \times 10^{-3}T$
980-1360 K: $\Delta Hf° = -22.371 - 0.265 \times 10^{-3}T - 0.609 \times 10^{-6}T^{2} + 198.550T^{-1}$
$\Delta Gf° = -22.371 + 0.265 \times 10^{-3}T\ln T + 0.609 \times 10^{-6}T^{2} + 99.275T^{-1} - 0.060 \times 10^{-3}T$
1360-1400 K: $\Delta Hf° = -22.344 - 0.036 \times 10^{-3}T - 1.045 \times 10^{-6}T^{2} + 145.150T^{-1}$
$\Delta Gf° = -22.344 + 0.036 \times 10^{-3}T\ln T + 1.045 \times 10^{-6}T^{2} + 72.575T^{-1} + 0.994 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Eremenko (140). Other data from Chart (77).

$Mn_3Si(c)$
Trimanganese Silicide
[Formation: $3Mn(c) + Si(c) = Mn_3Si(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	23.860	24.800	24.800	0	-25.700	-24.910	18.259
300	23.940	24.950	24.817	.040	-25.705	-24.910	18.147
400	26.890	32.270	25.770	2.600	-25.608	-24.652	13.469
500	28.930	38.500	27.720	5.390	-25.458	-24.428	10.677
600	30.600	43.930	29.980	8.370	-25.276	-24.244	8.831
700	32.110	48.760	32.317	11.510	-25.073	-24.093	7.522
800	33.520	53.140	34.653	14.790	-24.852	-23.972	6.549
900	34.880	57.170	36.937	18.210	-24.602	-23.882	5.799
980	35.944	60.181	38.713	21.038	-24.375	-23.810	5.310
980	35.944	60.181	38.713	21.038	-25.971	-23.810	5.310
1000	36.210	60.910	39.150	21.760	-25.916	-23.776	5.196

Phase change: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 24.111 + 12.448 \times 10^{-3}T - 3.518 \times 10^{5}T^{-2}$

$H° - H°_{298} = 24.111 \times 10^{-3}T + 6.224 \times 10^{-6}T^{2} + 3.518 \times 10^{2}T^{-1} - 8.922$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = -26.733 + 1.518 \times 10^{-3}T + 0.752 \times 10^{-6}T^{2} + 153.100T^{-1}$

$\Delta Gf° = -26.733 - 1.518 \times 10^{-3}T\ln T - 0.752 \times 10^{-6}T^{2} + 76.550T^{-1} + 14.127 \times 10^{-3}T$

980-1000 K: $\Delta Hf° = -25.476 - 5.025 \times 10^{-3}T + 4.181 \times 10^{-6}T^{2} + 413.500T^{-1}$

$\Delta Gf° = -25.476 + 5.025 \times 10^{-3}T\ln T - 4.181 \times 10^{-6}T^{2} + 206.750T^{-1} - 28.997 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Eremenko (140). Other data from Chart (77).

Mn_5Si_3(c,l)
Pentamanganese Trisilicide
[Formation: $5Mn(c,l) + 3Si(c,l) = Mn_5Si_3(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	46.710	57.100	57.100	0	-65.400	-66.995	49.108
300	46.800	57.390	57.100	.090	-65.397	-67.002	48.810
400	50.380	71.390	58.990	4.960	-65.308	-67.568	36.917
500	52.720	82.900	62.660	10.120	-65.276	-68.126	29.777
600	54.590	92.680	66.863	15.490	-65.332	-68.698	25.023
700	56.230	101.220	71.177	21.030	-65.475	-69.269	21.626
800	57.750	108.830	75.418	26.730	-65.680	-69.800	19.068
900	59.200	115.710	79.510	32.580	-65.940	-70.296	17.070
980	60.320	120.799	82.675	37.361	-66.164	-70.632	15.751
980	60.320	120.799	82.675	37.361	-68.824	-70.632	15.751
1000	60.600	122.020	83.450	38.570	-68.894	-70.684	15.448
1100	61.980	127.870	87.234	44.700	-69.200	-70.839	14.074
1200	63.330	133.320	90.845	50.970	-69.442	-71.014	12.933
1300	64.680	138.440	94.309	57.370	-69.622	-71.143	11.960
1360	65.478	141.374	96.323	61.270	-69.707	-71.154	11.434
1360	65.478	141.374	96.323	61.270	-72.242	-71.154	11.434
1400	66.010	143.280	97.637	63.900	-72.473	-71.129	11.104
1410	66.142	143.750	97.963	64.561	-72.530	-71.072	11.016
1410	66.142	143.750	97.963	64.561	-74.775	-71.072	11.016
1500	67.330	147.880	100.833	70.570	-75.462	-70.872	10.326
1517	67.556	148.640	101.365	71.717	-75.590	-70.773	10.196
1517	67.556	148.640	101.365	71.717	-90.000	-70.773	10.196
1573	68.300	151.100	103.092	75.520	-90.398	-70.029	9.730
1573	77.600	177.360	103.092	116.820	-49.098	-70.029	9.730
1600	77.600	178.680	104.361	118.910	-49.036	-70.396	9.616
1687	77.600	182.784	108.296	125.661	-48.828	-71.466	9.258
1687	77.600	182.784	108.296	125.661	-85.074	-71.466	9.258
1700	77.600	183.380	108.868	126.670	-85.017	-71.349	9.172
1800	77.600	187.820	113.137	134.430	-84.587	-70.547	8.565
1900	77.600	192.010	117.173	142.190	-84.157	-69.812	8.030
2000	77.600	196.000	121.025	149.950	-83.727	-69.047	7.545

Phase changes:
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.
1573 K, melting point of Mn_5Si_3; ΔH° = 41.300 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1573 K: $Cp^\circ = 48.126 + 12.944\times10^{-3}T - 4.682\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 48.126\times10^{-3}T + 6.472\times10^{-6}T^2 + 4.682\times10^{2}T^{-1} - 16.494$
1573-2000 K: $Cp^\circ = 77.600$
$H^\circ - H^\circ_{298} = 77.600\times10^{-3}T - 5.245$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf^\circ = -66.006 + 2.899\times10^{-3}T - 3.116\times10^{-6}T^2 + 5.700T^{-1}$
$\Delta Gf^\circ = -66.006 - 2.899\times10^{-3}T\ln T + 3.116\times10^{-6}T^2 + 2.850T^{-1} + 12.240\times10^{-3}T$
980-1360 K: $\Delta Hf^\circ = -63.911 - 8.006\times10^{-3}T + 2.599\times10^{-6}T^2 + 439.700T^{-1}$
$\Delta Gf^\circ = -63.911 + 8.006\times10^{-3}T\ln T - 2.599\times10^{-6}T^2 + 219.850T^{-1} - 59.632\times10^{-3}T$
1360-1410 K: $\Delta Hf^\circ = -63.775 - 6.861\times10^{-3}T + 0.419\times10^{-6}T^2 + 172.700T^{-1}$
$\Delta Gf^\circ = -63.775 + 6.861\times10^{-3}T\ln T - 0.419\times10^{-6}T^2 + 86.350T^{-1} - 54.363\times10^{-3}T$
1410-1517 K: $\Delta Hf^\circ = -62.514 - 9.806\times10^{-3}T + 0.744\times10^{-6}T^2 + 172.700T^{-1}$
$\Delta Gf^\circ = -62.514 + 9.806\times10^{-3}T\ln T - 0.744\times10^{-6}T^2 + 86.350T^{-1} - 76.155\times10^{-3}T$
1517-1573 K: $\Delta Hf^\circ = -66.285 - 23.911\times10^{-3}T + 5.419\times10^{-6}T^2 + 172.700T^{-1}$
$\Delta Gf^\circ = -66.285 + 23.911\times10^{-3}T\ln T - 5.419\times10^{-6}T^2 + 86.350T^{-1} - 169.889\times10^{-3}T$
1573-1687 K: $\Delta Hf^\circ = -55.036 + 5.563\times10^{-3}T - 1.053\times10^{-6}T^2 - 295.500T^{-1}$
$\Delta Gf^\circ = -55.036 - 5.563\times10^{-3}T\ln T + 1.053\times10^{-6}T^2 - 147.750T^{-1} + 29.825\times10^{-3}T$
1687-2000 K: $\Delta Hf^\circ = -92.323 + 4.300\times10^{-3}T$
$\Delta Gf^\circ = -92.323 - 4.300\times10^{-3}T\ln T + 44.267\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Eremenko (140). Other data from Chart (77).

MnSiO$_3$(c)
Manganese Silicate
[Formation: Mn(c,l) + Si(c,l) + 1.5O$_2$(g) = MnSiO$_3$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	20.709	21.300	21.300	0	-315.700	-296.512	217.346
300	20.799	21.428	21.301	.038	-315.703	-296.393	215.919
400	24.130	27.927	22.165	2.305	-315.660	-289.960	158.425
500	25.923	33.520	23.890	4.815	-315.490	-283.549	123.938
600	27.093	38.356	25.906	7.470	-315.282	-277.182	100.962
700	27.956	42.601	27.995	10.224	-315.068	-270.853	84.563
800	28.642	46.380	30.061	13.055	-314.857	-264.553	72.271
900	29.215	49.787	32.067	15.948	-314.655	-258.277	62.717
980	29.609	52.292	33.616	18.302	-314.493	-253.260	56.479
980	29.609	52.292	33.616	18.302	-315.025	-253.260	56.479
1000	29.707	52.891	33.996	18.895	-314.988	-252.004	55.075
1100	30.136	55.743	35.845	21.888	-314.796	-245.713	48.818
1200	30.516	58.382	37.615	24.921	-314.595	-239.451	43.609
1300	30.851	60.838	39.308	27.989	-314.387	-233.200	39.204
1360	31.029	62.235	40.289	29.846	-314.260	-229.443	36.871
1360	31.029	62.235	40.289	29.846	-314.767	-229.443	36.871
1400	31.148	63.136	40.929	31.090	-314.721	-226.936	35.426
1410	31.174	63.358	41.087	31.402	-314.709	-226.299	35.076
1410	31.174	63.358	41.087	31.402	-315.158	-226.299	35.076
1500	31.409	65.294	42.482	34.218	-315.095	-220.646	32.148
1517	31.448	65.648	42.740	34.752	-315.083	-219.567	31.632
1517	31.448	65.648	42.740	34.752	-317.965	-219.567	31.632
1600	31.636	67.328	43.972	37.370	-317.908	-214.179	29.255
1687	31.807	69.008	45.220	40.130	-317.841	-208.514	27.013
1687	31.807	69.008	45.220	40.130	-329.923	-208.514	27.013
1700	31.832	69.252	45.403	40.544	-329.904	-207.574	26.685
1800	31.997	71.077	46.779	43.736	-329.754	-200.377	24.329

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 27.035 + 3.164\times10^{-3}T - 6.462\times10^{5}T^{-2}$
$H° - H°_{298} = 27.035\times10^{-3}T + 1.582\times10^{-6}T^{2} + 6.462\times10^{2}T^{-1} - 10.368$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf° = -318.541 + 4.873\times10^{-3}T - 1.230\times10^{-6}T^{2} + 446.500T^{-1}$
$\Delta Gf° = -318.541 - 4.873\times10^{-3}T\ln T + 1.230\times10^{-6}T^{2} + 223.250T^{-1} + 98.773\times10^{-3}T$
980-1360 K: $\Delta Hf° = -318.122 + 2.692\times10^{-3}T - 0.087\times10^{-6}T^{2} + 533.300T^{-1}$
$\Delta Gf° = -318.122 - 2.692\times10^{-3}T\ln T + 0.087\times10^{-6}T^{2} + 266.650T^{-1} + 84.398\times10^{-3}T$
1360-1410 K: $\Delta Hf° = -318.095 + 2.921\times10^{-3}T - 0.523\times10^{-6}T^{2} + 479.900T^{-1}$
$\Delta Gf° = -318.095 - 2.921\times10^{-3}T\ln T + 0.523\times10^{-6}T^{2} + 239.950T^{-1} + 85.452\times10^{-3}T$
1410-1517 K: $\Delta Hf° = -317.842 + 2.332\times10^{-3}T - 0.458\times10^{-6}T^{2} + 479.900T^{-1}$
$\Delta Gf° = -317.842 - 2.332\times10^{-3}T\ln T + 0.458\times10^{-6}T^{2} + 239.950T^{-1} + 81.094\times10^{-3}T$
1517-1687 K: $\Delta Hf° = -318.597 - 0.489\times10^{-3}T + 0.477\times10^{-6}T^{2} + 479.900T^{-1}$
$\Delta Gf° = -318.597 + 0.489\times10^{-3}T\ln T - 0.477\times10^{-6}T^{2} + 239.950T^{-1} + 62.347\times10^{-3}T$
1687-1800 K: $\Delta Hf° = -331.026 - 0.910\times10^{-3}T + 0.828\times10^{-6}T^{2} + 578.400T^{-1}$
$\Delta Gf° = -331.026 + 0.910\times10^{-3}T\ln T - 0.828\times10^{-6}T^{2} + 289.200T^{-1} + 67.161\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from King (257). Low-temperature heat capacities and entropy at 298 K from Kelley (240). High-temperature data based on Southard (470).

Mn_2SiO_4(c,l)
Dimanganese Silicate
[Formation: $2Mn(c,l) + Si(c,l) + 2O_2(g) = Mn_2SiO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	30.745	37.380	37.380	0	-413.600	-389.620	285.595
300	30.864	37.571	37.381	.057	-413.602	-389.471	283.726
400	35.198	47.123	38.653	3.388	-413.502	-381.439	208.406
500	37.436	55.241	41.181	7.030	-413.264	-373.444	163.230
600	38.850	62.199	44.119	10.848	-413.012	-365.507	133.134
700	39.875	68.268	47.144	14.787	-412.784	-357.614	111.651
800	40.692	73.648	50.127	18.817	-412.591	-349.749	95.546
900	41.388	78.482	53.014	22.921	-412.435	-341.906	83.025
980	41.885	82.028	55.239	26.253	-412.326	-335.626	74.847
980	41.885	82.028	55.239	26.253	-413.390	-335.626	74.847
1000	42.009	82.875	55.783	27.092	-413.370	-334.045	73.005
1100	42.582	86.906	58.431	31.322	-413.265	-326.108	64.791
1200	43.121	90.635	60.963	35.607	-413.152	-318.207	57.953
1300	43.636	94.107	63.380	39.945	-413.028	-310.303	52.166
1360	43.935	96.083	64.779	42.573	-412.951	-305.542	49.099
1360	43.935	96.083	64.779	42.573	-413.965	-305.542	49.099
1400	44.134	97.359	65.692	44.334	-413.988	-302.356	47.199
1410	44.183	97.673	65.918	44.776	-413.994	-301.540	46.738
1410	44.183	97.673	65.918	44.776	-414.892	-301.540	46.738
1500	44.620	100.420	67.906	48.771	-415.022	-294.323	42.882
1517	44.701	100.923	68.273	49.530	-415.047	-292.937	42.202
1517	44.701	100.923	68.273	49.530	-420.811	-292.937	42.202
1600	45.097	103.315	70.029	53.257	-420.922	-285.925	39.055
1620	45.191	103.876	70.444	54.160	-420.945	-284.238	38.345
1620	59.000	116.987	70.444	75.400	-399.705	-284.238	38.345
1687	59.000	119.378	72.340	79.353	-398.860	-279.447	36.202
1687	59.000	119.378	72.340	79.353	-410.942	-279.447	36.202
1700	59.000	119.831	72.702	80.120	-410.770	-278.430	35.794
1800	59.000	123.203	75.414	86.020	-409.456	-270.674	32.864
1900	59.000	126.393	78.014	91.920	-408.154	-263.019	30.254
2000	59.000	129.420	80.510	97.820	-406.862	-255.398	27.908

Phase changes:
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.
1620 K, melting point of Mn_2SiO_4; ΔH° = 21.240 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1620 K: $Cp^\circ = 38.481 + 4.330\times10^{-3}T - 8.022\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 38.481\times10^{-3}T + 2.165\times10^{-6}T^2 + 8.022\times10^{2}T^{-1} - 14.356$
1620-2000 K: $Cp^\circ = 59.000$
$H^\circ - H^\circ_{298} = 59.000\times10^{-3}T - 20.180$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf^\circ = -417.308 + 7.066\times10^{-3}T - 2.606\times10^{-6}T^2 + 546.500T^{-1}$
$\Delta Gf^\circ = -417.308 - 7.066\times10^{-3}T\ln T + 2.606\times10^{-6}T^2 + 273.250T^{-1} + 129.275\times10^{-3}T$
980-1360 K: $\Delta Hf^\circ = -416.470 + 2.704\times10^{-3}T - 0.320\times10^{-6}T^2 + 720.100T^{-1}$
$\Delta Gf^\circ = -416.470 - 2.704\times10^{-3}T\ln T + 0.320\times10^{-6}T^2 + 360.050T^{-1} + 100.526\times10^{-3}T$
1360-1410 K: $\Delta Hf^\circ = -416.415 + 3.162\times10^{-3}T - 1.192\times10^{-6}T^2 + 613.300T^{-1}$
$\Delta Gf^\circ = -416.415 - 3.162\times10^{-3}T\ln T + 1.192\times10^{-6}T^2 + 306.650T^{-1} + 102.634\times10^{-3}T$
1410-1517 K: $\Delta Hf^\circ = -415.911 + 1.984\times10^{-3}T - 1.062\times10^{-6}T^2 + 613.300T^{-1}$
$\Delta Gf^\circ = -415.911 - 1.984\times10^{-3}T\ln T + 1.062\times10^{-6}T^2 + 306.650T^{-1} + 93.917\times10^{-3}T$
1517-1620 K: $\Delta Hf^\circ = -417.419 - 3.658\times10^{-3}T + 0.808\times10^{-6}T^2 + 613.300T^{-1}$
$\Delta Gf^\circ = -417.419 + 3.658\times10^{-3}T\ln T - 0.808\times10^{-6}T^2 + 306.650T^{-1} + 56.424\times10^{-3}T$
1620-1687 K: $\Delta Hf^\circ = -423.243 + 16.861\times10^{-3}T - 1.357\times10^{-6}T^2 - 188.900T^{-1}$
$\Delta Gf^\circ = -423.243 - 16.861\times10^{-3}T\ln T + 1.357\times10^{-6}T^2 - 94.450T^{-1} + 208.303\times10^{-3}T$
1687-2000 K: $\Delta Hf^\circ = -435.672 + 16.440\times10^{-3}T - 1.006\times10^{-6}T^2 - 90.400T^{-1}$
$\Delta Gf^\circ = -435.672 - 16.440\times10^{-3}T\ln T + 1.006\times10^{-6}T^2 - 45.200T^{-1} + 213.117\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Low-temperature heat capacities and entropy at 298 K from Robie (427). High-temperature data based on Christensen (92).

MnTe(c)
Manganese Telluride
[Reaction: $Mn(c) + 0.5Te_2(g) = MnTe(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	18.000	22.400	22.400	0	-45.765	-40.939	30.009
300	18.451	22.512	22.402	.033	-45.752	-40.911	29.803
305	20.315	22.831	22.408	.129	-45.709	-40.831	29.257
400	13.239	26.664	22.999	1.466	-45.411	-39.362	21.506
500	13.012	29.585	24.037	2.774	-45.249	-37.869	16.552
600	13.236	31.975	25.168	4.084	-45.137	-36.404	13.260
700	13.645	34.044	26.291	5.427	-45.041	-34.960	10.915

Phase change: 305 K, second order transition point of MnTe; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-305 K: $Cp° = -101.113 + 397.728\times10^{-3}T$
$H°-H°_{298} = -101.113\times10^{-3}T + 198.864\times10^{-6}T^2 + 12.469$
305-700 K: $Cp° = -25.178 + 50.780\times10^{-3}T + 27.912\times10^{5}T^{-2}$
$H°-H°_{298} = -25.178\times10^{-3}T + 25.390\times10^{-6}T^2 - 27.912\times10^{2}T^{-1} + 14.598$

Reaction equations (kcal/mol):

298.15-305 K: $\Delta Hr° = -30.002 - 111.050\times10^{-3}T + 196.861\times10^{-6}T^2 - 45.500T^{-1}$
$\Delta Gr° = -30.002 + 111.050\times10^{-3}T\ln T - 196.861\times10^{-6}T^2 - 22.750T^{-1} - 610.454\times10^{-3}T$
305-700 K: $\Delta Hr° = -27.874 - 35.116\times10^{-3}T + 23.386\times10^{-6}T^2 - 2836.700T^{-1}$
$\Delta Gr° = -27.874 + 35.116\times10^{-3}T\ln T - 23.386\times10^{-6}T^2 - 1418.350T^{-1} - 220.969\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (332). Low-temperature heat capacities and entropy at 298 K from Kelley (238). High-temperature data based on Gronvold (189).

$MnWO_4(c)$
Manganese Tungstate
[Formation: $Mn(c) + W(c) + 2O_2(g) = MnWO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	27.470	31.660	31.660	0	-318.000	-293.611	215.220
300	27.558	31.830	31.660	.051	-317.998	-293.459	213.782
400	30.839	40.263	32.788	2.990	-317.722	-285.315	155.887
500	32.672	47.357	35.013	6.172	-317.306	-277.258	121.188
600	33.934	53.431	37.588	9.506	-316.842	-269.296	98.090
700	34.927	58.739	40.239	12.950	-316.362	-261.410	81.615
800	35.776	63.459	42.852	16.486	-315.872	-253.599	69.279
900	36.542	67.718	45.381	20.103	-315.374	-245.840	59.697
980	37.113	70.854	47.334	23.049	-314.964	-239.674	53.449
980	37.113	70.854	47.334	23.049	-315.496	-239.674	53.449
1000	37.256	71.605	47.812	23.793	-315.395	-238.130	52.043
1100	37.937	75.188	50.140	27.553	-314.871	-230.411	45.778
1200*	38.594	78.518	52.368	31.380	-314.318	-222.772	40.572
1300	39.235	81.632	54.500	35.271	-313.734	-215.163	36.172
1360	39.612	83.411	55.737	37.636	-313.372	-210.604	33.843
1360	39.612	83.411	55.737	37.636	-313.879	-210.604	33.843
1400	39.864	84.563	56.544	39.226	-313.668	-207.572	32.403
1410	39.926	84.847	56.744	39.625	-313.615	-206.805	32.054
1410	39.926	84.847	56.744	39.625	-314.064	-206.805	32.054
1500	40.485	87.334	58.505	43.244	-313.610	-199.982	29.137

*Data extrapolated above 1100 K.

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 31.971 + 5.840x10^{-3}T - 5.549x10^{5}T^{-2}$
$H°- H°_{298} = 31.971x10^{-3}T + 2.920x10^{-6}T^{2} + 5.549x10^{2}T^{-1} - 11.653$

Formation equations (kcal/mol):

298.15-980 K: $ΔHf° = -321.167 + 6.058x10^{-3}T - 0.164x10^{-6}T^{2} + 410.100T^{-1}$
$ΔGf° = -321.167 - 6.058x10^{-3}TlnT + 0.164x10^{-6}T^{2} + 205.050T^{-1} + 124.583x10^{-3}T$
980-1360 K: $ΔHf° = -320.748 + 3.877x10^{-3}T + 0.979x10^{-6}T^{2} + 496.900T^{-1}$
$ΔGf° = -320.748 - 3.877x10^{-3}TlnT - 0.979x10^{-6}T^{2} + 248.450T^{-1} + 110.209x10^{-3}T$
1360-1410 K: $ΔHf° = -320.721 + 4.106x10^{-3}T + 0.543x10^{-6}T^{2} + 443.500T^{-1}$
$ΔGf° = -320.721 - 4.106x10^{-3}TlnT - 0.543x10^{-6}T^{2} + 221.750T^{-1} + 111.262x10^{-3}T$
1410-1500 K: $ΔHf° = -320.469 + 3.517x10^{-3}T + 0.608x10^{-6}T^{2} + 443.500T^{-1}$
$ΔGf° = -320.469 - 3.517x10^{-3}TlnT - 0.608x10^{-6}T^{2} + 221.750T^{-1} + 106.904x10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Amosse (10). Low-temperature heat capacities and entropy at 298 K from Landee (294). High-temperature data based on Yakoleva (536). Data extrapolated above 1100 K.

$Mn_{0.703}Zn_{0.0884}Ca_{0.2086}SiO_3$(fowlerite)
Fowlerite

[Formation: $0.703Mn(c,l) + 0.0884Zn(c,l,g) + 0.2086Ca(c,l,g) + Si(c,l) + 1.5O_2(g) = fowlerite(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	20.738	21.949	21.949	0	-329.910	-310.712	227.755
300	20.808	22.078	21.949	.039	-329.911	-310.592	226.263
400	23.332	28.442	22.799	2.257	-329.907	-304.153	166.179
500	24.994	33.835	24.481	4.677	-329.811	-297.721	130.132
600	26.454	38.522	26.439	7.250	-329.665	-291.317	106.111
692.73	27.848	42.421	28.321	9.767	-329.484	-285.407	90.042
692.73	27.848	42.421	28.321	9.767	-329.639	-285.407	90.042
700	27.957	42.712	28.469	9.970	-329.622	-284.943	88.962
720	28.258	43.504	28.876	10.532	-329.576	-283.666	86.103
720	28.258	43.504	28.876	10.532	-329.622	-283.666	86.103
800	29.462	46.544	30.493	12.841	-329.396	-278.572	76.101
900	30.770	50.093	32.475	15.856	-329.055	-272.236	66.107
980	31.470	52.747	34.023	18.350	-328.756	-267.192	59.586
980	31.470	52.747	34.023	18.350	-329.130	-267.192	59.586
1000	31.645	53.385	34.404	18.981	-329.055	-265.931	58.118
1100	31.945	56.419	36.269	22.165	-328.683	-259.637	51.584
1112	31.921	56.765	36.488	22.548	-328.641	-258.885	50.880
1112	31.921	56.765	36.488	22.548	-329.067	-258.885	50.880
1180	31.787	58.659	37.712	24.718	-328.782	-254.607	47.156
1180	31.787	58.659	37.712	24.718	-331.218	-254.607	47.156
1200	31.747	59.193	38.066	25.353	-331.135	-253.309	46.133
1300	31.473	61.722	39.790	28.511	-330.752	-246.843	41.498
1350	31.566	62.910	40.624	30.086	-330.576	-243.606	39.437

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
980 K, α - β transition point of Mn; ΔH° = 0.532 kca/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1350 K: $Cp° = 23.016 + 8.164\times10^{-3}T - 4.189\times10^{5}T^{-2}$
$H° - H°_{298} = 23.016\times10^{-3}T + 4.082\times10^{-6}T^{2} + 4.189\times10^{2}T^{-1} - 8.630$

Formation equations (kcal/mol):

298.15-692.73 K: $\Delta Hf° = -331.205 + 1.279\times10^{-3}T + 1.117\times10^{-6}T^{2} + 242.958T^{-1}$
$\Delta Gf° = -331.205 - 1.279\times10^{-3}T\ln T - 1.117\times10^{-6}T^{2} + 121.479T^{-1} + 74.986\times10^{-3}T$
692.73- 720 K: $\Delta Hf° = -331.271 + 1.066\times10^{-3}T + 1.240\times10^{-6}T^{2} + 241.844T^{-1}$
$\Delta Gf° = -331.271 - 1.066\times10^{-3}T\ln T - 1.240\times10^{-6}T^{2} + 120.922T^{-1} + 73.778\times10^{-3}T$
720-980 K: $\Delta Hf° = -331.634 + 1.888\times10^{-3}T + 0.746\times10^{-6}T^{2} + 229.120T^{-1}$
$\Delta Gf° = -331.634 - 1.888\times10^{-3}T\ln T - 0.746\times10^{-6}T^{2} + 114.560T^{-1} + 79.343\times10^{-3}T$
980-1112 K: $\Delta Hf° = -331.339 + 0.355\times10^{-3}T + 1.549\times10^{-6}T^{2} + 290.140T^{-1}$
$\Delta Gf° = -331.339 - 0.355\times10^{-3}T\ln T - 1.549\times10^{-6}T^{2} + 145.070T^{-1} + 69.238\times10^{-3}T$
1112-1180 K: $\Delta Hf° = -331.391 - 1.128\times10^{-3}T + 2.580\times10^{-6}T^{2} + 290.140T^{-1}$
$\Delta Gf° = -331.391 + 1.128\times10^{-3}T\ln T - 2.580\times10^{-6}T^{2} + 145.070T^{-1} + 60.032\times10^{-3}T$
1180-1350 K: $\Delta Hf° = -334.092 - 0.904\times10^{-3}T + 2.580\times10^{-6}T^{2} + 290.140T^{-1}$
$\Delta Gf° = -334.092 + 0.904\times10^{-3}T\ln T - 2.580\times10^{-6}T^{2} + 145.070T^{-1} + 63.905\times10^{-3}T$

Source: Data from Bennington (32).

MoB(c)
Molybdenum Boride
[Formation: $Mo(c) + B(\beta) = MoB(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	7.790	6.040	6.040	0	-29.600	-28.938	21.212
300	7.830	6.090	6.057	.010	-29.606	-28.938	21.081
400	9.470	8.600	6.375	.890	-29.630	-28.709	15.686
500	10.290	10.810	7.050	1.880	-29.654	-28.475	12.446
600	10.780	12.730	7.830	2.940	-29.694	-28.232	10.284
700	11.130	14.420	8.663	4.030	-29.759	-27.989	8.738
800	11.400	15.920	9.470	5.160	-29.824	-27.724	7.574
900	11.640	17.280	10.269	6.310	-29.902	-27.462	6.669
1000	11.860	18.520	11.030	7.490	-29.980	-27.184	5.941
1100	12.060	19.660	11.769	8.680	-30.078	-26.912	5.347
1200	12.260	20.720	12.470	9.900	-30.175	-26.616	4.847
1300	12.460	21.710	13.141	11.140	-30.284	-26.309	4.423
1400	12.670	22.640	13.790	12.390	-30.413	-26.003	4.059
1500	12.870	23.520	14.407	13.670	-30.545	-25.676	3.741
1600	13.090	24.360	15.004	14.970	-30.689	-25.359	3.464
1700	13.310	25.160	15.578	16.290	-30.848	-25.020	3.217
1800	13.530	25.920	16.126	17.630	-31.022	-24.650	2.993
1900	13.770	26.660	16.660	19.000	-31.205	-24.289	2.794
2000	14.010	27.370	17.180	20.380	-31.417	-23.937	2.616

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 10.645 + 1.566\times10^{-3}T - 2.953\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.645\times10^{-3}T + 0.783\times10^{-6}T^{2} + 2.953\times10^{2}T^{-1} - 4.234$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -30.409 + 1.545\times10^{-3}T - 1.094\times10^{-6}T^{2} + 133.000T^{-1}$

$\Delta Gf^\circ = -30.409 - 1.545\times10^{-3}T\ln T + 1.094\times10^{-6}T^{2} + 66.500T^{-1} + 12.664\times10^{-3}T$

Source: Data from Brewer (57) who estimated all except enthalpy of formation at 298 K.

$Mo_2B(c)$
Dimolybdenum Boride
[Formation: $2Mo(c) + B(\beta) = Mo_2B(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.950	12.580	12.580	0	-31.600	-30.846	22.610
300	14.010	12.670	12.580	.030	-31.597	-30.837	22.465
400	16.420	17.070	13.170	1.560	-31.558	-30.596	16.716
500	17.630	20.880	14.340	3.270	-31.469	-30.361	13.271
600	18.380	24.160	15.710	5.070	-31.394	-30.151	10.982
700	18.920	27.040	17.126	6.940	-31.316	-29.945	9.349
800	19.350	29.590	18.528	8.850	-31.250	-29.754	8.128
900	19.720	31.900	19.889	10.810	-31.177	-29.573	7.181
1000	20.070	33.990	21.190	12.800	-31.115	-29.393	6.424
1100	20.400	35.920	22.447	14.820	-31.067	-29.234	5.808
1200	20.720	37.710	23.643	16.880	-31.022	-29.064	5.293
1300	21.050	39.380	24.795	18.960	-31.006	-28.905	4.859
1400	21.370	40.950	25.886	21.090	-30.986	-28.732	4.485
1500	21.710	42.440	26.947	23.240	-30.997	-28.579	4.164
1600	22.050	43.850	27.956	25.430	-31.017	-28.422	3.882
1700	22.400	45.200	28.935	27.650	-31.063	-28.265	3.634
1800	22.760	46.490	29.873	29.910	-31.125	-28.083	3.410
1900	23.130	47.730	30.783	32.200	-31.221	-27.915	3.211
2000	23.510	48.920	31.655	34.530	-31.341	-27.741	3.031

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 17.879 + 2.698\text{x}10^{-3}T - 4.208\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 17.879\text{x}10^{-3}T + 1.349\text{x}10^{-6}T^{2} + 4.208\text{x}10^{2}T^{-1} - 6.862$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -33.826 + 4.402\text{x}10^{-3}T - 1.713\text{x}10^{-6}T^{2} + 317.700T^{-1}$
$\Delta Gf° = -33.826 - 4.402\text{x}10^{-3}T\ln T + 1.713\text{x}10^{-6}T^{2} + 158.850T^{-1} + 32.778\text{x}10^{-3}T$

Source: Data from Brewer (57) who estimated all except enthalpy of formation at 298 K.

MoC(γ)
γ-Molybdenum Carbide
[Formation: $Mo(c) + C(c) = MoC(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.380	8.760	8.760	0	-6.800	-6.960	5.102
300	7.400	8.810	8.760	.015	-6.800	-6.962	5.072
400	8.330	11.070	9.070	.800	-6.846	-7.012	3.831
500	9.100	13.010	9.660	1.675	-6.895	-7.043	3.078
600	9.750	14.730	10.363	2.620	-6.952	-7.066	2.574
700	10.280	16.270	11.099	3.620	-7.013	-7.080	2.210
800	10.710	17.670	11.833	4.670	-7.071	-7.084	1.935
900	11.060	18.960	12.560	5.760	-7.127	-7.089	1.721
1000	11.350	20.140	13.260	6.880	-7.184	-7.083	1.548
1100	11.600	21.230	13.930	8.030	-7.242	-7.053	1.401
1200	11.820	22.250	14.583	9.200	-7.308	-7.045	1.283
1300	12.030	23.200	15.208	10.390	-7.383	-7.018	1.180
1400	12.250	24.100	15.814	11.600	-7.463	-6.991	1.091
1500	12.510	24.960	16.400	12.840	-7.540	-6.963	1.014

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 8.285 + 3.100\times10^{-3}T - 1.626\times10^{5}T^{-2}$

$H°- H°_{298} = 8.285\times10^{-3}T + 1.550\times10^{-6}T^{2} + 1.626\times10^{2}T^{-1} - 3.153$

Formation equations (kcal/mol):

298.15-1500 K: $ΔHf° = -7.047 + 0.390\times10^{-3}T - 0.401\times10^{-6}T^{2} + 49.500T^{-1}$

$ΔGf° = -7.047 - 0.390\times10^{-3}T\ln T + 0.401\times10^{-6}T^{2} + 24.750T^{-1} + 2.113\times10^{-3}T$

Source: Data from Brewer (57).

$Mo_2C(c,l)$
Dimolybdenum Carbide
[Formation: $2Mo(c,l) + C(c) = Mo_2C(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	14.400	15.720	15.720	0	-11.900	-12.093	8.864
300	14.440	15.800	15.733	.020	-11.906	-12.099	8.814
400	16.040	20.200	16.300	1.560	-11.784	-12.172	6.651
500	17.020	23.900	17.460	3.220	-11.655	-12.283	5.369
600	17.740	27.060	18.793	4.960	-11.542	-12.414	4.522
700	18.340	29.860	20.203	6.760	-11.440	-12.585	3.929
800	18.860	32.340	21.565	8.620	-11.337	-12.754	3.484
900	19.300	34.580	22.891	10.520	-11.242	-12.940	3.142
1000	19.720	36.640	24.160	12.480	-11.129	-13.132	2.870
1100	20.100	38.540	25.376	14.480	-11.021	-13.320	2.646
1200	20.440	40.300	26.550	16.500	-10.935	-13.545	2.467
1300	20.760	41.940	27.663	18.560	-10.855	-13.755	2.312
1400	21.060	43.500	28.743	20.660	-10.776	-13.986	2.183
1500	21.330	44.960	29.773	22.780	-10.722	-14.215	2.071
1500	22.000	48.440	29.773	28.000	-5.502	-14.215	2.071
1600	22.200	49.880	31.005	30.200	-5.408	-14.829	2.025
1700	22.400	51.220	32.138	32.440	-5.324	-15.391	1.979
1800	22.600	52.500	33.233	34.680	-5.287	-15.983	1.941
1900	22.800	53.740	34.287	36.960	-5.265	-16.593	1.909
2000	23.000	54.920	35.300	39.240	-5.299	-17.209	1.880
2100	23.200	56.040	36.250	41.560	-5.351	-17.779	1.850
2200	23.400	57.120	37.175	43.880	-5.473	-18.374	1.825
2300	23.600	58.160	38.056	46.240	-5.619	-18.927	1.798
2400	23.800	59.180	38.930	48.600	-5.852	-19.544	1.780
2500	24.000	60.160	39.760	51.000	-6.131	-20.113	1.758
2600	24.200	61.100	40.562	53.400	-6.503	-20.660	1.737
2700	24.400	62.020	41.339	55.840	-6.930	-21.194	1.716
2795	24.590	62.850	42.044	58.160	-7.429	-21.654	1.693
2795	24.000	68.880	42.044	75.000	9.411	-21.654	1.693
2800	24.000	68.920	42.091	75.120	9.380	-21.708	1.694
2890	24.000	69.677	42.937	77.280	8.768	-22.692	1.716
2890	24.000	69.677	42.937	77.280	-6.786	-22.692	1.716
2900	24.000	69.760	43.029	77.520	-6.773	-22.749	1.714
3000	24.000	70.580	43.940	79.920	-6.646	-23.320	1.699

Phase changes: 1500 K, α - β transition point of Mo_2C; $\Delta H° = 5.220$ kcal/mol.
2795 K, melting point of Mo_2C; $\Delta H° = 16.840$ kcal/mol.
2890 K, melting point of Mo; $\Delta H° = 7.777$ kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 16.314 + 3.596\times10^{-3}T - 2.652\times10^{5}T^{-2}$
$H°-H°_{298} = 16.314\times10^{-3}T + 1.798\times10^{-6}T^2 + 2.652\times10^{2}T^{-1} - 5.913$
1500-2795 K: $Cp° = 18.990 + 2.002\times10^{-3}T$
$H°-H°_{298} = 18.990\times10^{-3}T + 1.001\times10^{-6}T^2 - 2.737$
2795-3000 K: $Cp° = 24.000$
$H°-H°_{298} = 24.000\times10^{-3}T + 7.920$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = -13.695 + 4.042\times10^{-3}T - 1.338\times10^{-6}T^2 + 211.300T^{-1}$
$\Delta Gf° = -13.695 - 4.042\times10^{-3}T\ln T + 1.338\times10^{-6}T^2 + 105.650T^{-1} + 26.814\times10^{-3}T$
1500-2000 K: $\Delta Hf° = -10.519 + 6.718\times10^{-3}T - 2.135\times10^{-6}T^2 - 53.900T^{-1}$
$\Delta Gf° = -10.519 - 6.718\times10^{-3}T\ln T + 2.135\times10^{-6}T^2 - 26.950T^{-1} + 43.131\times10^{-3}T$
2000-2795 K: $\Delta Hf° = -8.527 + 4.595\times10^{-3}T - 1.503\times10^{-6}T^2 - 601.600T^{-1}$
$\Delta Gf° = -8.527 - 4.595\times10^{-3}T\ln T + 1.503\times10^{-6}T^2 - 300.800T^{-1} + 27.330\times10^{-3}T$
2795-2890 K: $\Delta Hf° = 2.130 + 9.605\times10^{-3}T - 2.504\times10^{-6}T^2 - 601.600T^{-1}$
$\Delta Gf° = 2.130 - 9.605\times10^{-3}T\ln T + 2.504\times10^{-6}T^2 - 300.800T^{-1} + 60.477\times10^{-3}T$
2890-3000 K: $\Delta Hf° = -11.138 + 1.979\times10^{-3}T - 0.134\times10^{-6}T^2 - 720.000T^{-1}$
$\Delta Gf° = -11.138 - 1.979\times10^{-3}T\ln T + 0.134\times10^{-6}T^2 - 360.000T^{-1} + 11.153\times10^{-3}T$

Source: Data from Brewer (57).

$Mo(CO)_6(g)$
Molybdenum Hexacarbonyl (ideal gas)
[Formation: $Mo(c) + 6C(c) + 3O_2(g) = Mo(CO)_6(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	50.333	120.077	120.077	0	-218.900	-206.372	151.273
300	50.449	120.389	120.079	.093	-218.881	-206.295	150.284
350	53.026	128.367	120.696	2.685	-218.312	-204.238	127.530
400	55.015	135.582	122.112	5.388	-217.767	-202.263	110.510
450	56.638	142.158	123.987	8.177	-217.270	-200.361	97.307
500	58.027	148.199	126.109	11.045	-216.812	-198.505	86.765
550	59.254	153.788	128.370	13.980	-216.406	-196.689	78.156
600	60.360	158.991	130.708	16.970	-216.039	-194.913	70.996

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 51.504 + 17.680 \times 10^{-3}T - 5.727 \times 10^{5}T^{-2}$
$H° - H°_{298} = 51.504 \times 10^{-3}T + 8.840 \times 10^{-6}T^{2} + 5.727 \times 10^{2}T^{-1} - 18.063$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = -218.526 + 4.329 \times 10^{-3}T + 1.550 \times 10^{-6}T^{2} - 537.500T^{-1}$
$\Delta Gf° = -218.526 - 4.329 \times 10^{-3}T\ln T - 1.550 \times 10^{-6}T^{2} - 268.750T^{-1} + 68.915 \times 10^{-3}T$

Source: Data from Pilcher (401).

$MoN_{0.5}(c)$
Molybdenum Nitride
[Formation: $Mo(c) + 0.25N_2(g) = MoN_{0.5}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.630	7.550	7.550	0	-9.750	-6.547	4.799
300	7.660	7.600	7.550	.015	-9.749	-6.527	4.755
400	8.690	9.960	7.872	.835	-9.691	-5.464	2.985
500	9.370	11.970	8.490	1.740	-9.568	-4.416	1.930
600	9.890	13.730	9.222	2.705	-9.406	-3.402	1.239
700	10.320	15.290	9.976	3.720	-9.210	-2.413	.753
800	10.710	16.690	10.728	4.770	-8.995	-1.455	.398
900	11.050	17.970	11.459	5.860	-8.754	-.524	.127
1000	11.350	19.150	12.170	6.980	-8.498	.376	-.082
1100	11.630	20.250	12.859	8.130	-8.229	1.246	-.247
1200	11.880	21.270	13.520	9.300	-7.957	2.093	-.381
1300	12.110	22.230	14.153	10.500	-7.674	2.920	-.491
1400	12.310	23.140	14.769	11.720	-7.391	3.716	-.580
1500	12.490	23.990	15.350	12.960	-7.107	4.507	-.657

<u>Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations</u>:

298.15-1500 K: $Cp° = 8.822 + 2.618x10^{-3}T - 1.753x10^{5}T^{-2}$

$H°-H°_{298} = 8.822x10^{-3}T + 1.309x10^{-6}T^2 + 1.753x10^{2}T^{-1} - 3.335$

<u>Formation equations (kcal/mol)</u>:

298.15-1500 K: $ΔHf° = -11.381 + 2.816x10^{-3}T - 0.023x10^{-6}T^2 + 236.475T^{-1}$

$ΔGf° = -11.381 - 2.816x10^{-3}T\ln T + 0.023x10^{-6}T^2 + 118.238T^{-1} + 30.917x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mah (<u>316</u>). Other data from Brewer (<u>57</u>).

$MoO_2Cl_2(g)$
Molybdenum Dioxychloride (ideal gas)
[Formation: $Mo(c) + O_2(g) + Cl_2(g) = MoO_2Cl_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	20.368	80.705	80.705	0	-151.300	-142.821	104.689
300	20.405	80.831	80.705	.038	-151.301	-142.768	104.005
400	22.034	86.942	81.527	2.166	-151.300	-139.922	76.449
500	23.081	91.979	83.129	4.425	-151.232	-137.082	59.918
600	23.773	96.253	84.970	6.770	-151.136	-134.262	48.904
700	24.244	99.955	86.851	9.173	-151.026	-131.457	41.042
800	24.576	103.215	88.696	11.615	-150.917	-128.671	35.151
900	24.817	106.125	90.475	14.085	-150.810	-125.896	30.571
1000	24.996	108.749	92.173	16.576	-150.710	-123.135	26.911
1100	25.133	111.138	93.790	19.083	-150.623	-120.381	23.917
1200	25.239	113.330	95.329	21.601	-150.551	-117.635	21.424
1300	25.323	115.353	96.791	24.130	-150.495	-114.893	19.315
1400	25.390	117.232	98.186	26.665	-150.459	-112.156	17.508
1500	25.446	118.986	99.515	29.207	-150.442	-109.423	15.943
1600	25.491	120.630	100.784	31.754	-150.446	-106.688	14.573
1700	25.529	122.176	101.997	34.305	-150.473	-103.949	13.363
1800	25.561	123.637	103.159	36.860	-150.525	-101.212	12.289
1900	25.588	125.019	104.273	39.417	-150.607	-98.469	11.326
2000	25.612	126.331	105.342	41.977	-150.719	-95.721	10.460

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.132 + 1.034x10^{-3}T - 3.620x10^{5}T^{-2}$

$H°- H°_{298} = 24.132x10^{-3}T + 0.517x10^{-6}T^{2} + 3.620x10^{2}T^{-1} - 8.455$

Formation equations (kcal/mol):

298.15-2000 K: $ΔHf° = -153.323 + 3.698x10^{-3}T - 1.259x10^{-6}T^{2} + 307.700T^{-1}$

$ΔGf° = -153.323 - 3.698x10^{-3}TlnT + 1.259x10^{-6}T^{2} + 153.850T^{-1} + 54.188x10^{-3}T$

Source: Data are those estimated by JANAF (127).

$MoOF_4(g)$
Molybdenum Oxytetrafluoride (ideal gas)
[Formation: $Mo(c) + 0.5O_2(g) + 2F_2(g) = MoOF_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	23.121	78.992	78.992	0	-300.000	-285.317	209.140
300	23.185	79.135	78.992	.043	-300.003	-285.226	207.785
400	25.929	86.213	79.938	2.510	-300.016	-280.293	153.143
500	27.631	92.196	81.808	5.194	-299.912	-275.373	120.364
600	28.720	97.337	83.979	8.015	-299.753	-270.481	98.521
700	29.445	101.822	86.213	10.926	-299.565	-265.615	82.928
800	29.948	105.789	88.418	13.897	-299.366	-260.782	71.241
900	30.308	109.338	90.548	16.911	-299.159	-255.968	62.157
1000	30.575	112.546	92.590	19.956	-298.958	-251.183	54.895
1100	30.776	115.470	94.539	23.024	-298.766	-246.413	48.957
1200	30.932	118.155	96.397	26.109	-298.585	-241.663	44.012
1300	31.055	120.636	98.168	29.209	-298.418	-236.924	39.830
1400	31.154	122.941	99.855	32.320	-298.270	-232.201	36.248
1500	31.234	125.093	101.467	35.439	-298.141	-227.488	33.145
1600	31.301	127.111	103.007	38.566	-298.030	-222.780	30.430
1700	31.356	129.011	104.482	41.699	-297.941	-218.078	28.036
1800	31.402	130.804	105.895	44.837	-297.879	-213.382	25.908
1900	31.442	132.503	107.251	47.979	-297.843	-208.688	24.004
2000	31.476	134.117	108.555	51.125	-297.839	-203.999	22.292

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 29.521 + 1.394\times10^{-3}T - 6.059\times10^{5}T^{-2}$

$H°-H°_{298} = 29.521\times10^{-3}T + 0.697\times10^{-6}T^{2} + 6.059\times10^{2}T^{-1} - 10.896$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -302.730 + 4.513\times10^{-3}T - 1.087\times10^{-6}T^{2} + 441.500T^{-1}$

$\Delta Gf° = -302.730 - 4.513\times10^{-3}T\ln T + 1.087\times10^{-6}T^{2} + 220.750T^{-1} + 81.308\times10^{-3}T$

Source: Data from JANAF (127) who estimated enthalpy of formation at 298 K and most molecular constants.

$MoSe_2(c)$
Molybdenum Diselenide
[Reaction: $Mo(c) + Se_2(g) = MoSe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15	16.850	21.290	21.290	0	-71.300	-58.253	42.700
300	16.870	21.390	21.290	.030	-71.299	-58.172	42.378
400*	17.800	26.390	21.965	1.770	-71.141	-53.820	29.405
500	18.260	30.420	23.260	3.580	-70.946	-49.507	21.639
600	18.540	33.780	24.747	5.420	-70.742	-45.244	16.480
700	18.730	36.650	26.250	7.280	-70.529	-41.011	12.804
800	18.880	39.160	27.710	9.160	-70.306	-36.806	10.055
900	19.000	41.390	29.101	11.060	-70.069	-32.628	7.923
1000	19.100	43.400	30.440	12.960	-69.838	-28.492	6.227
1100	19.190	45.220	31.693	14.880	-69.596	-24.355	4.839
1200	19.270	46.900	32.900	16.800	-69.362	-20.263	3.690
1300	19.350	48.440	34.032	18.730	-69.130	-16.171	2.718
1400	19.420	49.880	35.116	20.670	-68.898	-12.114	1.891
1500	19.490	51.220	36.147	22.610	-68.678	-8.069	1.176

*Data extrapolated above 340 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 18.680 + 0.596 \times 10^{-3}T - 1.788 \times 10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.680 \times 10^{-3}T + 0.298 \times 10^{-6}T^{2} + 1.788 \times 10^{2}T^{-1} - 6.196$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta Hr^\circ = -72.932 + 3.639 \times 10^{-3}T - 0.568 \times 10^{-6}T^{2} + 178.100T^{-1}$

$\Delta Gr^\circ = -72.932 - 3.639 \times 10^{-3}T\ln T + 0.568 \times 10^{-6}T^{2} + 89.050T^{-1} + 68.796 \times 10^{-3}T$

Source: Data from Brewer (57) who extrapolated above 340 K.

$Mo_3Se_4(c)$
Trimolybdenum Tetraselenide
[Reaction: $3Mo(c) + 2Se_2(g) = Mo_3Se_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	39.350	51.700	51.700	0	-147.000	-121.583	89.121
300	39.380	51.940	51.707	.070	-146.999	-121.428	88.459
400	40.770	63.480	53.255	4.090	-146.730	-112.938	61.706
500	41.630	72.680	56.260	8.210	-146.447	-104.525	45.687
600	42.290	80.330	59.647	12.410	-146.144	-96.171	35.030
700	42.860	86.890	63.076	16.670	-145.815	-87.857	27.430
800	43.370	92.650	66.425	20.980	-145.468	-79.600	21.745
900	43.850	97.780	69.624	25.340	-145.093	-71.389	17.335
1000	44.320	102.430	72.680	29.750	-144.691	-63.233	13.819
1100	44.770	106.670	75.579	34.200	-144.281	-55.100	10.947
1200	45.210	110.590	78.340	38.700	-143.851	-47.013	8.562
1300	45.650	114.220	80.958	43.240	-143.422	-38.949	6.548
1400	46.080	117.620	83.456	47.830	-142.979	-30.937	4.829
1500	46.510	120.820	85.847	52.460	-142.538	-22.961	3.345
1600	46.940	123.830	88.124	57.130	-142.096	-15.003	2.049
1700	47.370	126.690	90.308	61.850	-141.655	-7.042	.905

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1700 K: $Cp° = 40.340 + 4.174x10^{-3}T - 1.987x10^{5}T^{-2}$

$H°- H°_{298} = 40.340x10^{-3}T + 2.087x10^{-6}T^{2} + 1.987x10^{2}T^{-1} - 12.879$

Reaction equations (kcal/mol):

298.15-1700 K: $\Delta Hr° = -149.540 + 5.881x10^{-3}T - 0.830x10^{-6}T^{2} + 256.500T^{-1}$

$\Delta Gr° = -149.540 - 5.881x10^{-3}T\ln T + 0.830x10^{-6}T^{2} + 128.250T^{-1} + 125.586x10^{-3}T$

Source: Data from Brewer (57) who estimated all except enthalpy of formation at 298 K.

$MoSi_2(c)$
Molybdenum Disilicide
[Formation: $Mo(c) + 2Si(c,l) = MoSi_2(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^\circ_{298})/T$	$H°-H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.300	15.540	15.540	0	-31.400	-31.308	22.949
300	15.327	15.635	15.542	.028	-31.401	-31.308	22.807
400	16.376	20.204	16.156	1.619	-31.411	-31.279	17.090
500	17.015	23.931	17.349	3.291	-31.438	-31.239	13.655
600	17.493	27.077	18.715	5.017	-31.481	-31.200	11.364
700	17.894	29.804	20.108	6.787	-31.530	-31.149	9.725
800	18.255	32.217	21.474	8.594	-31.582	-31.088	8.493
900	18.592	34.387	22.790	10.437	-31.638	-31.022	7.533
1000	18.914	36.363	24.051	12.312	-31.689	-30.936	6.761
1100	19.227	38.180	25.254	14.219	-31.740	-30.873	6.134
1200	19.533	39.866	26.402	16.157	-31.788	-30.792	5.608
1300	19.835	41.442	27.499	18.126	-31.834	-30.708	5.162
1400	20.133	42.923	28.549	20.124	-31.881	-30.611	4.779
1500	20.429	44.322	29.554	22.152	-31.928	-30.542	4.450
1600	20.723	45.650	30.519	24.210	-31.972	-30.450	4.159
1687	20.978	46.754	31.328	26.024	-32.013	-30.324	3.928
1687	20.978	46.754	31.328	26.024	-56.177	-30.324	3.928
1700	21.016	46.915	31.446	26.297	-56.166	-30.117	3.872
1800	21.307	48.124	32.339	28.413	-56.078	-28.581	3.470
1900	21.598	49.284	33.201	30.558	-55.986	-27.057	3.112
2000	21.888	50.399	34.032	32.733	-55.889	-25.547	2.792

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.215 + 2.856\times10^{-3}T - 1.570\times10^{5}T^{-2}$

$H°-H^\circ_{298} = 16.215\times10^{-3}T + 1.428\times10^{-6}T^{2} + 1.570\times10^{2}T^{-1} - 5.488$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -31.567 + 0.480\times10^{-3}T - 0.459\times10^{-6}T^{2} + 19.200T^{-1}$

$\Delta Gf° = -31.567 - 0.480\times10^{-3}T\ln T + 0.459\times10^{-6}T^{2} + 9.600T^{-1} + 3.359\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -56.425 - 0.362\times10^{-3}T + 0.243\times10^{-6}T^{2} + 216.200T^{-1}$

$\Delta Gf° = -56.425 + 0.362\times10^{-3}T\ln T - 0.243\times10^{-6}T^{2} + 108.100T^{-1} + 12.987\times10^{-3}T$

Source: Data from Brewer (57).

$Mo_3Si(c)$
Trimolybdenum Silicide
[Formation: $3Mo(c) + Si(c,l) = Mo_3Si(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	22.227	25.160	25.160	0	-28.300	-28.333	20.768
300	22.236	25.298	25.160	.042	-28.300	-28.333	20.640
400	22.741	31.763	26.038	2.290	-28.320	-28.346	15.487
500	23.266	36.894	27.714	4.590	-28.387	-28.342	12.388
600	23.799	41.182	29.609	6.944	-28.480	-28.326	10.318
700	24.335	44.891	31.534	9.350	-28.576	-28.292	8.833
800	24.874	48.176	33.412	11.811	-28.667	-28.244	7.716
900	25.413	51.137	35.220	14.325	-28.750	-28.187	6.845
1000	25.954	53.842	36.949	16.893	-28.820	-28.114	6.144
1100	26.495	56.341	38.599	19.516	-28.886	-28.047	5.572
1200	27.036	58.670	40.177	22.192	-28.948	-27.966	5.093
1300	27.577	60.855	41.683	24.923	-29.012	-27.882	4.687
1400	28.119	62.919	43.128	27.708	-29.077	-27.788	4.338
1500	28.660	64.877	44.512	30.547	-29.148	-27.707	4.037
1600	29.202	66.744	45.844	33.440	-29.221	-27.607	3.771
1687	29.674	68.303	46.963	36.001	-29.297	-27.497	3.562
1687	29.674	68.303	46.963	36.001	-41.379	-27.497	3.562
1700	29.744	68.531	47.127	36.387	-41.382	-27.386	3.521
1800	30.286	70.246	48.363	39.389	-41.414	-26.557	3.224
1900	30.828	71.898	49.559	42.444	-41.468	-25.732	2.960
2000	31.370	73.493	50.716	45.554	-41.542	-24.908	2.722

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 20.524 + 5.422\times10^{-3}T + 0.077\times10^{5}T^{-2}$

$H°-H°_{298} = 20.524\times10^{-3}T + 2.711\times10^{-6}T^{2} - 0.077\times10^{2}T^{-1} - 6.334$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -28.944 + 1.714\times10^{-3}T - 1.195\times10^{-6}T^{2} + 71.400T^{-1}$

$\Delta Gf° = -28.944 - 1.714\times10^{-3}T\ln T + 1.195\times10^{-6}T^{2} + 35.700T^{-1} + 11.059\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -41.373 + 1.293\times10^{-3}T - 0.844\times10^{-6}T^{2} + 169.900T^{-1}$

$\Delta Gf° = -41.373 - 1.293\times10^{-3}T\ln T + 0.844\times10^{-6}T^{2} + 84.950T^{-1} + 15.873\times10^{-3}T$

Source: Data from Brewer (57).

$Mo_5Si_3(c)$
Pentamolybdenum Trisilicide
[Formation: $5Mo(c) + 3Si(c,l) = Mo_5Si_3(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	43.098	49.680	49.680	0	-74.200	-74.775	54.811
300	43.153	49.947	49.680	.080	-74.202	-74.780	54.477
400	45.384	62.695	51.403	4.517	-74.221	-74.977	40.965
500	46.866	72.990	54.724	9.133	-74.278	-75.153	32.849
600	48.053	81.642	58.507	13.881	-74.371	-75.326	27.437
700	49.101	89.130	62.360	18.739	-74.471	-75.475	23.564
800	50.075	95.750	66.126	23.699	-74.571	-75.607	20.655
900	51.006	101.702	69.754	28.753	-74.672	-75.731	18.390
1000	51.910	107.123	73.224	33.899	-74.760	-75.823	16.571
1100	52.797	112.113	76.537	39.134	-74.856	-75.948	15.089
1200	53.671	116.744	79.696	44.458	-74.954	-76.039	13.848
1300	54.538	121.074	82.714	49.868	-75.069	-76.127	12.798
1400	55.398	125.148	85.602	55.365	-75.198	-76.189	11.894
1500	56.254	128.999	88.367	60.948	-75.349	-76.292	11.116
1600	57.106	132.657	91.022	66.616	-75.515	-76.350	10.429
1687	57.845	135.700	93.248	71.616	-75.690	-76.328	9.888
1687	57.845	135.700	93.248	71.616	-111.936	-76.328	9.888
1700	57.955	136.144	93.574	72.369	-111.938	-76.041	9.776
1800	58.803	139.481	96.033	78.207	-111.970	-73.920	8.975
1900	59.649	142.683	98.405	84.129	-112.043	-71.807	8.260
2000	60.493	145.764	100.696	90.136	-112.156	-69.704	7.617

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 43.829 + 8.368\times10^{-3}T - 2.868\times10^{5}T^{-2}$
$H°- H°_{298} = 43.829\times10^{-3}T + 4.184\times10^{-6}T^{2} + 2.868\times10^{2}T^{-1} - 14.401$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -76.378 + 4.907\times10^{-3}T - 2.794\times10^{-6}T^{2} + 287.300T^{-1}$
$\Delta Gf° = -76.378 - 4.907\times10^{-3}T\ln T + 2.794\times10^{-6}T^{2} + 143.650T^{-1} + 30.885\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -113.666 + 3.644\times10^{-3}T - 1.741\times10^{-6}T^{2} + 582.800T^{-1}$
$\Delta Gf° = -113.666 - 3.644\times10^{-3}T\ln T + 1.741\times10^{-6}T^{2} + 291.400T^{-1} + 45.327\times10^{-3}T$

Source: Data from Brewer (57).

$MoTe_2(c)$
Molybdenum Ditelluride
[Reaction: $Mo(c) + Te_2(g) = MoTe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	18.370	27.550	27.550	0	-56.830	-44.555	32.659
300	18.390	27.660	27.560	.030	-56.827	-44.483	32.406
400*	19.240	33.090	28.290	1.920	-56.403	-40.430	22.090
500	19.640	37.430	29.690	3.870	-55.956	-36.482	15.946
600	19.880	41.030	31.297	5.840	-55.524	-32.630	11.885
700	20.030	44.110	32.910	7.840	-55.090	-28.848	9.007
800	20.130	46.790	34.478	9.850	-54.675	-25.127	6.864
900	20.210	49.170	35.981	11.870	-54.275	-21.460	5.211
1000	20.280	51.300	37.410	13.890	-53.903	-17.837	3.898
1100	20.330	53.230	38.757	15.920	-53.550	-14.238	2.829
1200	20.380	55.010	40.043	17.960	-53.218	-10.683	1.946
1260	20.410	56.000	40.778	19.180	-53.038	-8.559	1.484

*Data extrapolated above 340 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1260 K: $Cp° = 20.190 + 0.258\text{x}10^{-3}T - 1.689\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 20.190\text{x}10^{-3}T + 0.129\text{x}10^{-6}T^{2} + 1.689\text{x}10^{2}T^{-1} - 6.598$

Reaction equations (kcal/mol):

298.15-1260 K: $\Delta Hr° = -59.518 + 7.214\text{x}10^{-3}T - 1.649\text{x}10^{-6}T^{2} + 203.900T^{-1}$

$\Delta Gr° = -59.518 - 7.214\text{x}10^{-3}T\ln T + 1.649\text{x}10^{-6}T^{2} + 101.950T^{-1} + 89.650\text{x}10^{-3}T$

Source: Data from Brewer (57) who extrapolated above 340 K.

Mo_3Te_4(c)
Trimolybdenum Tetratelluride
[Reaction: 3Mo(c) + $2Te_2$(g) = Mo_3Te_4(c)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	42.920	64.000	64.000	0	-115.660	-91.722	67.233
300	42.940	64.270	64.003	.080	-115.645	-91.577	66.713
400	43.950	76.780	65.705	4.430	-114.814	-83.678	45.719
500	44.490	86.650	68.930	8.860	-113.997	-75.980	33.210
600	44.850	94.790	72.590	13.320	-113.238	-68.449	24.932
700	45.120	101.730	76.273	17.820	-112.507	-61.045	19.059
800	45.350	107.770	79.832	22.350	-111.816	-53.740	14.681
900	45.550	113.120	83.242	26.890	-111.175	-46.525	11.298
1000	45.730	117.930	86.480	31.450	-110.581	-39.383	8.607
1100	45.900	122.300	89.536	36.040	-110.029	-32.277	6.413
1200	46.060	126.300	92.442	40.630	-109.553	-25.231	4.595
1300	46.220	129.990	95.182	45.250	-109.128	-18.214	3.062
1400	46.370	133.420	97.791	49.880	-108.773	-11.235	1.754
1500	46.520	136.620	100.273	54.520	-108.470	-4.283	.624
1600	46.670	139.630	102.643	59.180	-108.196	2.641	-.361

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 44.513 + 1.392x10^{-3}T - 1.788x10^{5}T^{-2}$
$H°- H°_{298} = 44.513x10^{-3}T + 0.696x10^{-6}T^{2} + 1.788x10^{2}T^{-1} - 13.933$

Reaction equations (kcal/mol):

298.15-1600 K: $ΔHr° = -120.562 + 14.184x10^{-3}T - 4.045x10^{-6}T^{2} + 308.000T^{-1}$
$ΔGr° = -120.562 - 14.184x10^{-3}T\ln T + 4.045x10^{-6}T^{2} + 154.000T^{-1} + 174.609x10^{-3}T$

Source: Data from Brewer (57) who estimated all except enthalpy of formation at 298 K.

NH(g)
Nitrogen Monohydride (ideal gas), Imidogen
[Formation: $0.5N_2(g) + 0.5H_2(g) = NH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	6.966	43.294	43.294	0	90.000	88.567	-64.921
300	6.966	43.337	43.294	.013	90.000	88.558	-64.514
400	6.973	45.342	43.567	.710	90.001	88.078	-48.123
500	6.994	46.900	44.084	1.408	89.998	87.596	-38.288
600	7.041	48.179	44.664	2.109	89.993	87.116	-31.731
700	7.119	49.270	45.246	2.817	89.987	86.637	-27.049
800	7.223	50.227	45.810	3.534	89.979	86.159	-23.537
900	7.343	51.085	46.349	4.262	89.972	85.682	-20.806
1000	7.471	51.865	46.862	5.003	89.966	85.205	-18.621
1100	7.600	52.583	47.349	5.757	89.964	84.730	-16.834
1200	7.726	53.250	47.814	6.523	89.962	84.254	-15.345
1300	7.845	53.873	48.256	7.302	89.962	83.780	-14.084
1400	7.958	54.458	48.678	8.092	89.964	83.304	-13.004
1500	8.062	55.011	49.082	8.893	89.966	82.828	-12.068
1600	8.158	55.534	49.469	9.704	89.971	82.352	-11.249
1700	8.247	56.032	49.841	10.524	89.976	81.875	-10.526
1800	8.330	56.505	50.198	11.353	89.982	81.399	-9.883
1900	8.407	56.958	50.542	12.190	89.990	80.921	-9.308
2000	8.478	57.391	50.874	13.034	89.998	80.444	-8.790

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.301 + 1.146 \times 10^{-3}T + 0.288 \times 10^{5}T^{-2}$

$H° - H°_{298} = 6.301 \times 10^{-3}T + 0.573 \times 10^{-6}T^{2} - 0.288 \times 10^{2}T^{-1} - 1.833$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 90.105 - 0.185 \times 10^{-3}T + 0.069 \times 10^{-6}T^{2} - 16.600T^{-1}$

$\Delta Gf° = 90.105 + 0.185 \times 10^{-3}T\ln T - 0.069 \times 10^{-6}T^{2} - 8.300T^{-1} - 6.100 \times 10^{-3}T$

Source: Data from Chase (80).

$NH_2(g)$
Nitrogen Dihydride (ideal gas), Amidogen
[Formation: $0.5N_2(g) + H_2(g) = NH_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.024	46.510	46.510	0	45.500	47.761	-35.009
300	8.027	46.560	46.510	.015	45.495	47.774	-34.803
400	8.221	48.894	46.826	.827	45.265	48.570	-26.537
500	8.493	50.756	47.432	1.662	45.049	49.421	-21.602
600	8.805	52.332	48.120	2.527	44.858	50.314	-18.326
700	9.143	53.714	48.823	3.424	44.689	51.237	-15.997
800	9.492	54.958	49.513	4.356	44.544	52.182	-14.255
900	9.842	56.096	50.183	5.322	44.419	53.144	-12.905
1000	10.181	57.151	50.827	6.324	44.316	54.119	-11.828
1100	10.503	58.137	51.448	7.358	44.230	55.103	-10.948
1200	10.802	59.064	52.045	8.423	44.159	56.095	-10.216
1300	11.079	59.939	52.617	9.518	44.103	57.094	-9.598
1400	11.333	60.770	53.171	10.638	44.056	58.093	-9.069
1500	11.566	61.560	53.704	11.784	44.021	59.098	-8.610
1600	11.781	62.313	54.219	12.951	43.993	60.103	-8.210
1700	11.981	63.033	54.716	14.139	43.972	61.112	-7.856
1800	12.167	63.724	55.198	15.347	43.959	62.119	-7.542
1900	12.344	64.386	55.664	16.572	43.952	63.129	-7.261
2000	12.511	65.024	56.117	17.815	43.951	64.138	-7.009
2100	12.672	65.638	56.555	19.074	43.955	65.148	-6.780
2200	12.826	66.231	56.981	20.349	43.966	66.155	-6.572
2300	12.975	66.804	57.396	21.639	43.983	67.165	-6.382
2400	13.120	67.360	57.800	22.944	44.007	68.173	-6.208
2500	13.261	67.898	58.193	24.263	44.035	69.179	-6.048

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 7.504 + 2.570\text{x}10^{-3}T - 0.219\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 7.504\text{x}10^{-3}T + 1.285\text{x}10^{-6}T^{2} + 0.219\text{x}10^{2}T^{-1} - 2.425$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 45.966 - 2.210\text{x}10^{-3}T + 0.572\text{x}10^{-6}T^{2} + 42.350T^{-1}$

$\Delta Gf° = 45.966 + 2.210\text{x}10^{-3}T\ln T - 0.572\text{x}10^{-6}T^{2} + 21.175T^{-1} - 6.644\text{x}10^{-3}T$

2000-2500 K: $\Delta Hf° = 47.303 - 3.275\text{x}10^{-3}T + 0.838\text{x}10^{-6}T^{2} - 507.600T^{-1}$

$\Delta Gf° = 47.303 + 3.275\text{x}10^{-3}T\ln T - 0.838\text{x}10^{-6}T^{2} - 253.800T^{-1} - 14.798\text{x}10^{-3}T$

Source: Data from Chase (80).

$NH_3(g)$
Ammonia (ideal gas)
[Formation: $0.5N_2(g) + 1.5H_2(g) = NH_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.521	46.048	46.048	0	-10.980	-3.929	2.880
300	8.533	46.101	46.048	.016	-10.990	-3.886	2.831
400	9.253	48.650	46.390	.904	-11.491	-1.440	.787
500	10.050	50.801	47.063	1.869	-11.927	1.124	-.491
600	10.825	52.702	47.847	2.913	-12.289	3.769	-1.373
700	11.557	54.426	48.666	4.032	-12.587	6.470	-2.020
800	12.245	56.015	49.486	5.223	-12.826	9.210	-2.516
900	12.894	57.495	50.295	6.480	-13.015	11.975	-2.908
1000	13.502	58.885	51.085	7.800	-13.159	14.760	-3.226
1100	14.068	60.199	51.854	9.179	-13.264	17.557	-3.488
1200	14.591	61.446	52.603	10.612	-13.334	20.363	-3.709
1300	15.071	62.633	53.328	12.096	-13.375	23.174	-3.896
1400	15.510	63.766	54.034	13.625	-13.391	25.985	-4.056
1500	15.909	64.850	54.719	15.197	-13.384	28.798	-4.196
1600	16.271	65.889	55.385	16.806	-13.358	31.607	-4.317
1700	16.599	66.885	56.032	18.450	-13.316	34.419	-4.425
1800	16.896	67.842	56.661	20.125	-13.260	37.225	-4.520
1900	17.165	68.763	57.275	21.828	-13.193	40.028	-4.604
2000	17.408	69.650	57.872	23.557	-13.116	42.826	-4.680

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.917 + 5.384x10^{-3}T - 0.890x10^{5}T^{-2}$

$H°-H°_{298} = 7.917x10^{-3}T + 2.692x10^{-6}T^{2} + 0.890x10^{2}T^{-1} - 2.898$

Formation equations (kcal/mol):

298.15-2000 K: $ΔHf° = -10.034 - 5.026x10^{-3}T + 1.769x10^{-6}T^{2} + 117.700T^{-1}$

$ΔGf° = -10.034 + 5.026x10^{-3}T\ln T - 1.769x10^{-6}T^{2} + 58.850T^{-1} - 8.294x10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (94). Other data from Chase (80).

$ND_3(g)$
Trideutero-Ammonia (ideal gas)
[Formation: $0.5N_2(g) + 1.5D_2(g) = ND_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	9.136	48.715	48.715	0	-14.000	-6.218	4.558
300	9.155	48.771	48.715	.017	-14.009	-6.170	4.495
400	10.259	51.556	49.086	.988	-14.434	-3.489	1.906
500	11.323	53.961	49.827	2.067	-14.756	-.714	.312
600	12.302	56.113	50.698	3.249	-14.988	2.117	-.771
700	13.195	58.078	51.614	4.525	-15.144	4.981	-1.555
800	14.003	59.894	52.537	5.886	-15.239	7.864	-2.148
900	14.723	61.585	53.448	7.323	-15.285	10.755	-2.612
1000	15.358	63.170	54.343	8.827	-15.292	13.647	-2.983
1100	15.912	64.661	55.215	10.391	-15.267	16.539	-3.286
1200	16.394	66.066	56.060	12.007	-15.215	19.431	-3.539
1300	16.813	67.395	56.881	13.668	-15.144	22.316	-3.752
1400	17.177	68.655	57.678	15.368	-15.056	25.193	-3.933
1500	17.495	69.851	58.450	17.102	-14.956	28.065	-4.089
1600	17.773	70.989	59.198	18.866	-14.843	30.931	-4.225
1700	18.016	72.074	59.924	20.655	-14.724	33.786	-4.343
1800	18.231	73.110	60.628	22.468	-14.596	36.637	-4.448
1900	18.420	74.101	61.311	24.301	-14.463	39.480	-4.541
2000	18.587	75.050	61.975	26.151	-14.326	42.315	-4.624

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.892 + 5.196x10^{-3}T - 2.049x10^{5}T^{-2}$

$H°- H°_{298} = 9.892x10^{-3}T + 2.598x10^{-6}T^{2} + 2.049x10^{2}T^{-1} - 3.867$

Formation equations (kcal/mol):

298.15-2000 K: $ΔHf° = -14.149 - 2.763x10^{-3}T + 1.360x10^{-6}T^{2} + 254.000T^{-1}$

$ΔGf° = -14.149 + 2.763x10^{-3}T\ln T - 1.360x10^{-6}T^{2} + 127.000T^{-1} + 9.838x10^{-3}T$

Source: Data from Chase (80) who estimated all except enthalpy of formation at 298 K.

$N_2H_2(g)$
Dinitrogen Dihydride (ideal gas), Diimide
[Formation: $N_2(g) + H_2(g) = N_2H_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.376	52.155	52.155	0	50.636	58.037	-42.541
300	8.388	52.207	52.155	.016	50.626	58.083	-42.313
400	9.263	54.732	52.494	.895	50.114	60.647	-33.136
500	10.341	56.913	53.163	1.875	49.692	63.332	-27.682
600	11.429	58.895	53.955	2.964	49.368	66.091	-24.073
700	12.459	60.735	54.795	4.158	49.133	68.898	-21.510
800	13.412	62.462	55.646	5.453	48.979	71.733	-19.596
900	14.290	64.093	56.495	6.838	48.894	74.583	-18.111
1000	15.096	65.641	57.333	8.308	48.871	77.438	-16.924
1100	15.836	67.115	58.155	9.856	48.905	80.295	-15.953
1200	16.516	68.523	58.961	11.474	48.987	83.145	-15.143
1300	17.138	69.870	59.749	13.157	49.113	85.988	-14.456
1400	17.708	71.161	60.518	14.900	49.279	88.818	-13.865
1500	18.226	72.401	61.270	16.697	49.480	91.635	-13.351
1600	18.694	73.592	62.003	18.543	49.713	94.436	-12.899
1700	19.114	74.738	62.718	20.434	49.974	97.226	-12.499
1800	19.488	75.842	63.418	22.364	50.259	99.995	-12.141
1900	19.818	76.904	64.099	24.330	50.566	102.751	-11.819
2000	20.106	77.928	64.765	26.326	50.889	105.489	-11.527

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.568 + 7.192\text{x}10^{-3}T - 1.187\text{x}10^{5}T^{-2}$

$H°-H°_{298} = 7.568\text{x}10^{-3}T + 3.596\text{x}10^{-6}T^{2} + 1.187\text{x}10^{2}T^{-1} - 2.974$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 51.537 - 5.405\text{x}10^{-3}T + 2.588\text{x}10^{-6}T^{2} + 143.100T^{-1}$

$\Delta Gf° = 51.537 + 5.405\text{x}10^{-3}T\ln T - 2.588\text{x}10^{-6}T^{2} + 71.550T^{-1} - 9.030\text{x}10^{-3}T$

Source: Data from Gurvich (194).

$N_2H_4(l,g)$
Hydrazine
[Formation: $N_2(g) + 2H_2(g) = N_2H_4(l,g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.623	29.050	29.050	0	12.100	35.694	-26.164
300	23.650	29.196	29.050	.044	12.105	35.840	-26.109
386.9	25.400	35.415	29.806	2.170	12.420	42.676	-24.106
386.9	14.413	60.486	29.806	11.870	22.120	42.676	-24.106
400	14.747	60.971	30.816	12.062	22.038	43.374	-23.698
500	16.861	64.498	37.204	13.647	21.522	48.772	-21.318
600	18.538	67.726	42.026	15.420	21.182	54.256	-19.762
700	19.910	70.690	45.913	17.344	20.975	59.786	-18.666
800	21.081	73.427	49.183	19.395	20.871	65.339	-17.850
900	22.111	75.970	52.019	21.556	20.851	70.900	-17.217
1000	23.030	78.348	54.534	23.814	20.898	76.458	-16.710
1100	23.854	80.583	56.802	26.159	21.003	82.009	-16.293
1200	24.592	82.690	58.872	28.582	21.154	87.551	-15.945
1300	25.252	84.685	60.782	31.074	21.343	93.077	-15.647
1400	25.842	86.579	62.558	33.630	21.566	98.586	-15.390
1500	26.367	88.380	64.219	36.241	21.814	104.079	-15.164
1600	26.836	90.097	65.784	38.901	22.084	109.551	-14.964
1700	27.254	91.737	67.263	41.606	22.372	115.012	-14.786
1800	27.626	93.305	68.666	44.350	22.674	120.452	-14.625
1900	27.960	94.808	70.003	47.130	22.989	125.876	-14.479
2000	28.258	96.250	71.280	49.941	23.312	131.282	-14.346
2100	28.525	97.635	72.501	52.781	23.644	136.674	-14.224
2200	28.766	98.968	73.675	55.645	23.979	142.044	-14.111
2300	28.982	100.251	74.802	58.533	24.321	147.406	-14.007
2400	29.177	101.489	75.889	61.441	24.666	152.754	-13.910
2500	29.354	102.684	76.937	64.368	25.013	158.080	-13.819

Phase change: 386.9 K, melting point of N_2H_4; ΔH° = 9.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-386.9 K: $Cp° = 18.062 + 18.652 \times 10^{-3}T$
$H°- H°_{298} = 18.062 \times 10^{-3}T + 9.326 \times 10^{-6}T^2 - 6.214$
386.9-2500 K: $Cp° = 18.500 + 5.146 \times 10^{-3}T - 9.098 \times 10^{5}T^{-2}$
$H°- H°_{298} = 18.500 \times 10^{-3}T + 2.573 \times 10^{-6}T^2 + 9.098 \times 10^{2}T^{-1} + 1.976$

Formation equations (kcal/mol):

298.15-386.9 K: $\Delta Hf° = 11.668 - 1.367 \times 10^{-3}T + 7.899 \times 10^{-6}T^2 + 40.900T^{-1}$
$\Delta Gf° = 11.668 + 1.367 \times 10^{-3}T\ln T - 7.899 \times 10^{-6}T^2 + 20.450T^{-1} + 74.919 \times 10^{-3}T$
386.9-2000 K: $\Delta Hf° = 19.858 - 0.929 \times 10^{-3}T + 1.146 \times 10^{-6}T^2 + 950.700T^{-1}$
$\Delta Gf° = 19.858 + 0.929 \times 10^{-3}T\ln T - 1.146 \times 10^{-6}T^2 + 475.350T^{-1} + 50.709 \times 10^{-3}T$
2000-2500 K: $\Delta Hf° = 22.532 - 3.057 \times 10^{-3}T + 1.679 \times 10^{-6}T^2 - 149.200T^{-1}$
$\Delta Gf° = 22.532 + 3.057 \times 10^{-3}T\ln T - 1.679 \times 10^{-6}T^2 - 74.600T^{-1} + 34.400 \times 10^{-3}T$

Source: Data from JANAF (127).

$NH_4Al(SO_4)_2(c)$
Ammonium Aluminum Sulfate

[Reaction: $0.5N_2(g) + 2H_2(g) + Al(c) + 4O_2(g) + S_2(g) = NH_4Al(SO_4)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	54.114	51.715	51.715	0	-593.110	-506.382	371.184
300	54.315	52.050	51.717	.100	-593.120	-505.844	368.502
400	65.333	69.620	54.035	6.234	-592.958	-476.751	260.481
500	69.816	84.730	58.700	13.015	-592.302	-447.766	195.716
600	72.512	97.714	64.147	20.140	-591.452	-418.936	152.595
650	73.552	103.560	66.957	23.792	-590.993	-404.578	136.030

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-650 K: $Cp° = 85.078 - 9.650x10^{-3}T - 24.967x10^{5}T^{-2}$

$H°- H°_{298} = 85.078x10^{-3}T - 4.825x10^{-6}T^{2} + 24.967x10^{2}T^{-1} - 33.311$

Reaction equations (kcal/mol):

298.15-650 K: $\Delta Hr° = -608.006 + 27.052x10^{-3}T - 10.017x10^{-6}T^{2} + 2301.950T^{-1}$

$\Delta Gr° = -608.006 - 27.052x10^{-3}T\ln T + 10.017x10^{-6}T^{2} + 1150.975T^{-1} + 479.048x10^{-3}T$

Source: Data from DeKock (113).

$NH_4Al(SO_4)_2 \cdot 12H_2O(c)$
Ammonium Aluminum Sulfate Dodecahydrate
[Reaction: $0.5N_2(g) + 14H_2(g) + Al(c) + 10O_2(g) + S_2(g) = NH_4Al(SO_4)_2 \cdot 12H_2O(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	162.962	166.600	166.600	0	-1451.130	-1199.338	879.127
300	163.740	167.610	166.603	.302	-1451.172	-1197.775	872.568
350	183.761	194.379	168.670	8.998	-1451.712	-1155.485	721.508
367.13	190.175	203.313	170.080	12.201	-1451.693	-1140.987	679.212

Phase changes: 367.13 K, melting point of $NH_4Al(SO_4)_2 \cdot 12H_2O$; ΔH° = 29.160 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-367.13 K: $Cp° = 87.218 + 310.982 \times 10^{-3}T - 15.090 \times 10^{5}T^{-2}$

$H° - H°_{298} = 87.218 \times 10^{-3}T + 155.491 \times 10^{-6}T^{2} + 15.090 \times 10^{2}T^{-1} - 44.887$

Reaction equations (kcal/mol):

298.15-367.13 K: $\Delta Hr° = -1440.610 - 91.659 \times 10^{-3}T + 142.253 \times 10^{-6}T^{2} + 1241.050T^{-1}$

$\Delta Gr° = -1440.610 + 91.659 \times 10^{-3}T\ln T - 142.253 \times 10^{-6}T^{2} + 620.525T^{-1} + 322.423 \times 10^{-3}T$

Source: Data from DeKock (113).

$NH_4Br(c)$
Ammonium Bromide
[Formation: $0.5N_2(g) + 2H_2(g) + 0.5Br_2(l,g) = NH_4Br(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	20.889	26.580	26.580	0	-64.730	-41.800	30.640
300	20.949	26.709	26.582	.038	-64.741	-41.658	30.348
332.6	21.543	28.901	26.704	.731	-64.906	-39.141	25.719
332.6	21.543	28.901	26.704	.731	-68.439	-39.141	25.719
400	22.770	33.040	27.433	2.243	-68.394	-33.209	18.144
412.66*	22.880	33.760	27.624	2.532	-68.381	-32.099	17.000
412.66	18.800	35.839	27.624	3.390	-67.523	-32.099	17.000
500	20.239	39.579	29.389	5.095	-67.732	-24.578	10.743
540	20.660	41.150	30.196	5.915	-67.791	-21.120	8.548

*Bartell gives α value of 5000 cal/mol•K for heat capacity at 412.66 K.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
412.66 K, II - I transition point of NH_4Br; ΔH° = 0.858 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-412.66 K: $Cp° = 28.966 - 7.276x10^{-3}T - 5.251x10^{5}T^{-2}$
$H°- H°_{298} = 28.966x10^{-3}T - 3.638x10^{-6}T^2 + 5.251x10^{2}T^{-1} - 10.074$
412.66-540 K: $Cp° = 12.508 + 5.370x10^{-3}T$
$H°- H°_{298} = 12.508x10^{-3}T + 7.685x10^{-6}T^2 - 3.080$

Formation equations (kcal/mol):

298.15-332.6 K: $ΔHf° = -67.314 + 3.750x10^{-3}T - 4.720x10^{-6}T2 + 562.050T^{-1}$
$ΔGf° = -67.314 - 3.750x10^{-3}TlnT + 4.720x10^{-6}T2 + 281.025T^{-1} + 102.371X10^{-3}T$
332.6-412.66 K: $ΔHf° = -72.314 + 8.330x10^{-3}T - 4.798x10^{-6}T2 + 546.350T^{-1}$
$ΔGf° = -72.314 - 8.330x10^{-3}TlnT + 4.798x10^{-6}T2 + 273.165T^{-1} + 144.049X10^{-3}T$
412.66-540 K: $ΔHf° = -65.320 - 8.128x10^{-3}T + 6.525x10^{-6}T2 + 21.250T^{-1}$
$ΔGf° = -65.320 + 8.128x10^{-3}TlnT - 6.525x10^{-6}T2 + 10.625T^{-1} + 34.194X10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data from Bartell (24).

$NH_4Cl(c)$
Ammonium Chloride
[Formation: $0.5N_2(g) + 2H_2(g) + 0.5Cl_2(g) = NH_4Cl(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	20.400	22.710	22.710	0	-75.330	-48.725	35.716
300	20.460	22.840	22.710	.040	-75.330	-48.559	35.375
350	22.010	26.110	22.967	1.100	-75.343	-44.097	27.535
400	23.440	29.140	23.540	2.240	-75.282	-39.631	21.653
450	24.940	31.990	24.323	3.450	-75.158	-35.183	17.087
457	25.160	32.370	24.449	3.620	-75.140	-34.563	16.529
457	19.770	34.690	24.449	4.680	-74.080	-34.563	16.529
500	21.130	36.530	25.410	5.560	-74.138	-30.843	13.481
550	22.710	38.620	26.529	6.650	-74.141	-26.520	10.538
600	24.290	40.660	27.610	7.830	-74.059	-22.187	8.081

Phase change: 457 K, α - β transition point of NH_4Cl; ΔH° = 1.060 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-457 K: $Cp° = 15.896 + 21.602x10^{-3}T - 1.721x10^{5}T^{-2}$
$H°- H°_{298} = 15.896x10^{-3}T + 10.801x10^{-6}T^{2} + 1.721x10^{2}T^{-1} - 6.277$
457-600 K: $Cp° = 5.292 + 31.672x10^{-3}T$
$H°- H°_{298} = 5.292x10^{-3}T + 15.836x10^{-6}T^{2} - 1.046$

Formation equations (kcal/mol):

298.15-457 K: $ΔHf° = -75.374 - 4.688x10^{-3}T + 9.625x10^{-6}T^{2} + 174.900T^{-1}$
$ΔGf° = -75.374 + 4.688x10^{-3}TlnT - 9.625x10^{-6}T^{2} + 87.450T^{-1} + 64.559x10^{-3}T$
457-600 K: $ΔHf° = -70.143 - 15.292x10^{-3}T + 14.660x10^{-6}T^{2} + 2.800T^{-1}$
$ΔGf° = -70.143 + 15.292x10^{-3}TlnT - 14.660x10^{-6}T^{2} + 1.400T^{-1} - 9.121x10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Parker (392). Other data based on Amitin (8), Arell (12), Callanan (65), Chihara (88), and Popov (405).

$NH_4ClO_4(c)$
Ammonium Perchlorate
[Formation: $0.5N_2(g) + 2H_2(g) + 0.5Cl_2(g) + 2O_2(g) = NH_4ClO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	30.610	44.020	44.020	0	-70.580	-21.107	15.471
300	30.700	44.210	44.020	.060	-70.586	-20.797	15.150
350	32.500	49.080	44.394	1.640	-70.783	-12.482	7.794
400	33.970	53.520	45.270	3.300	-70.917	-4.147	2.266
450	35.550	57.610	46.410	5.040	-70.989	4.207	-2.043
500	37.690	61.460	47.720	6.870	-70.986	12.565	-5.492
513	38.380	62.440	48.091	7.360	-70.973	14.732	-6.276
513*	33.000	66.860	48.091	9.630	-68.703	14.732	-6.276
550	33.000	69.160	49.433	10.850	-68.848	20.754	-8.247
600	33.000	72.030	51.197	12.500	-69.057	28.910	-10.530

*Heat capacity of $NH_4ClO_4(\beta)$ estimated.

Phase change: 513 K, α - β transition point of NH_4Cl; ΔH° = 2.270 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-513 K: $Cp° = 22.879 + 29.636x10^{-3}T - 0.982x10^{5}T^{-2}$
$H°- H°_{298} = 22.879x10^{-3}T + 14.818x10^{-6}T^{2} + 0.982x10^{2}T^{-1} - 8.468$
513-600 K: $Cp° = 33.000$
$H°- H°_{298} = 33.000x10^{-3}T - 7.299$

Formation equations (kcal/mol):

298.15-513 K: $ΔHf° = -68.112 - 12.165x10^{-3}T + 12.635x10^{-6}T^{2} + 10.600T^{-1}$
$ΔGf° = -68.112 + 12.165x10^{-3}TlnT - 12.635x10^{-6}T^{2} + 5.300T^{-1} + 92.052x10^{-3}T$
513-600 K: $ΔHf° = -66.943 - 2.044x10^{-3}T - 2.183x10^{-6}T^{2} - 87.600T^{-1}$
$ΔGf° = -66.943 + 2.044x10^{-3}TlnT + 2.183x10^{-6}T^{2} - 43.800T^{-1} + 145.516x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from Westrum (529). High-temperature data based on Rajeshwar (412). Heat capacity of $NH_4ClO_4(\beta)$ estimated.

$NH_4F(c,l)$
Ammonium Fluoride
[Formation: $0.5N_2(g) + 2H_2(g) + 0.5F_2(g) = NH_4F(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.600	17.201	17.201	0	-111.750	-84.225	61.738
300	15.676	17.298	17.201	.029	-111.760	-84.055	61.233
400	19.866	22.382	17.867	1.806	-112.104	-74.756	40.844
500	24.063	27.265	19.261	4.002	-112.060	-65.417	28.593
511	24.517	27.794	19.438	4.270	-112.030	-64.390	27.539
511	27.010	33.687	19.438	7.281	-109.019	-64.390	27.539
600	27.010	38.024	21.882	9.685	-108.549	-56.657	20.637
700	27.010	42.187	24.493	12.386	-108.039	-48.049	15.001
760	27.010	44.408	25.979	14.006	-107.745	-42.920	12.342

Phase change: 511 K, melting point of NH_4F; ΔH° = 3.011 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-511 K: $Cp° = 3.106 + 41.900x10^{-3}T$
$H°- H°_{298} = 3.106x10^{-3}T + 20.950x10^{-6}T^2 - 2.788$
511-760 K: $Cp° = 27.010$
$H°- H°_{298} = 27.010x10^{-3}T - 6.521$

Formation equations (kcal/mol):

298.15-511 K: $\Delta Hf° = -108.296 - 17.319x10^{-3}T + 19.731x10^{-6}T^2 - 13.300T^{-1}$
$\Delta Gf° = -108.296 + 17.319x10^{-3}TlnT - 19.731x10^{-6}T^2 - 6.650T^{-1} - 11.982x10^{-3}T$
511-760 K: $\Delta Hf° = -112.029 + 6.585x10^{-3}T - 1.220x10^{-6}T^2 - 13.300T^{-1}$
$\Delta Gf° = -112.029 - 6.585x10^{-3}TlnT + 1.220x10^{-6}T^2 - 6.650T^{-1} + 133.693x10^{-3}T$

Source: Data from Gurvich (194).

NH_4HF_2(c,l)
Ammonium Hydrogen Fluoride
[Formation: $0.5N_2(g) + 2.5H_2(g) + F_2(g) = NH_4HF_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	25.570	27.610	27.610	0	-193.600	-157.305	115.306
300	25.730	27.770	27.613	.047	-193.606	-157.081	114.432
399.6*	36.000	36.470	28.727	3.094	-193.400	-144.957	79.279
399.6	36.000	47.890	28.727	7.658	-188.836	-144.957	79.279
400	33.610	47.930	28.750	7.672	-188.834	-144.915	79.177
440	34.900	51.190	30.642	9.041	-188.620	-140.533	69.802

*Carling (70) gives a value of $6x10^4$ cal/mol·K for heat capacity at 399.6 K.

Phase change: 399.6 K, melting point of NH_4HF_2; ΔH° = 4.564 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-399.6 K: $Cp^\circ = -6.334 + 105.572x10^{-3}T$

$H^\circ - H^\circ_{298} = -6.334x10^{-3}T + 52.786x10^{-6}T^2 - 2.804$

399.6-440 K: $Cp^\circ = 50.339 - 38.370x10^{-3}T$

$H^\circ - H^\circ_{298} = 50.339x10^{-3}T - 19.185x10^{-6}T^2 - 9.394$

Formation equations (kcal/mol):

298.15-399.6 K: $\Delta Hf^\circ = -187.763 - 34.240x10^{-3}T + 51.270x10^{-6}T^2 - 55.300T^{-1}$

$\Delta Gf^\circ = -187.763 + 34.240x10^{-3}T\ln T - 51.270x10^{-6}T^2 - 27.650T^{-1} - 77.332x10^{-3}T$

399.6-440 K: $\Delta Hf^\circ = -194.354 + 22.433x10^{-3}T - 20.701x10^{-6}T^2 - 55.300T^{-1}$

$\Delta Gf^\circ = -194.354 - 22.433x10^{-3}T\ln T + 20.701x10^{-6}T^2 - 27.650T^{-1} + 249.898x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Bendaoud (27). Low-temperature heat capacities and entropy at 298 K from Burney (63). High-temperature date from Carling (70).

$NH_4I(c)$
Ammonium Iodide
[Formation: $0.5N_2(g) + 2H_2(g) + 0.5I_2(c,l,g) = NH_4I(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.540	28.000	28.000	0	-48.140	-26.918	19.731
300	19.570	28.121	28.001	.036	-48.148	-26.787	19.514
386.8	21.046	33.270	28.622	1.798	-48.497	-20.558	11.616
386.8	21.046	33.270	28.622	1.798	-50.352	-20.558	11.616
400	21.270	33.980	28.788	2.077	-50.430	-19.540	10.676
458.4	22.269	36.945	29.639	3.349	-50.742	-15.007	7.155
458.4	22.269	36.945	29.639	3.349	-55.752	-15.007	7.155
500	22.980	38.910	30.330	4.290	-55.725	-11.310	4.943
600	24.680	43.251	32.129	6.673	-55.548	-2.442	.890
700	26.400	47.184	34.003	9.227	-55.210	6.385	-1.993
800	26.130	50.822	35.881	11.953	-54.719	15.153	-4.140

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 14.381 + 17.154\times10^{-3}T + 0.039\times10^{5}T^{-2}$
$H° - H°_{298} = 14.381\times10^{-3}T + 8.577\times10^{-6}T^2 - 0.039\times10^{2}T^{-1} - 5.037$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -46.393 - 8.228\times10^{-3}T + 6.699\times10^{-6}T^2 + 33.050T^{-1}$
$\Delta Gf° = -46.393 + 8.228\times10^{-3}T\ln T - 6.699\times10^{-6}T^2 + 16.525T^{-1} + 20.250\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -47.121 - 11.430\times10^{-3}T + 7.445\times10^{-6}T^2 + 33.050T^{-1}$
$\Delta Gf° = -47.121 + 11.430\times10^{-3}T\ln T - 7.445\times10^{-6}T^2 + 16.525T^{-1} + 3.343\times10^{-3}T$
458.4-800 K: $\Delta Hf° = -54.477 - 6.260\times10^{-3}T + 7.411\times10^{-6}T^2 + 25.400T^{-1}$
$\Delta Gf° = -54.477 + 6.260\times10^{-3}T\ln T - 7.411\times10^{-6}T^2 + 12.700T^{-1} + 51.074\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (513). Other data are those estimated by JANAF (127).

$NH_4NO_3(c,l)$
Ammonium Nitrate
[Formation: $N_2(g) + 2H_2(g) + 1.5O_2(g) = NH_4NO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	33.241	36.044	36.044	0	-87.380	-43.955	32.220
300	33.377	36.250	36.050	.060	-87.379	-43.688	31.826
305.38	33.764	36.848	36.062	.240	-87.367	-42.905	30.705
305.38	28.528	38.177	36.062	.646	-86.961	-42.905	30.705
357.25	30.946	42.840	36.712	2.189	-87.047	-35.413	21.664
357.25	35.208	43.741	36.712	2.511	-86.725	-35.413	21.664
399	36.668	47.662	37.637	4.000	-86.557	-29.418	16.113
399	38.121	50.319	37.637	5.060	-85.497	-29.418	16.113
400	38.169	50.416	37.671	5.098	-85.491	-29.278	15.997
442.85	39.500	54.369	39.097	6.763	-85.190	-23.271	11.484
442.85	38.480	57.530	39.097	8.163	-83.790	-23.271	11.484
500	38.480	62.202	41.478	10.362	-83.424	-15.485	6.769
600	38.480	69.218	45.535	14.210	-82.821	-1.956	.712
700	38.480	75.150	49.353	18.058	-82.271	11.478	-3.584
800	38.480	80.288	52.906	21.906	-81.775	24.836	-6.785
900	38.480	84.820	56.204	25.754	-81.329	38.135	-9.260

Phase changes: 305.38 K, IV - III transition point of NH_4NO_3; ΔH° = 0.406 kcal/mol.
357.25 K, III - II transition point of NH_4NO_3; ΔH° = 0.322 kcal/mol.
399 K, II - I transition point of NH_4NO_3; ΔH° = 1.060 kcal/mol.
442.85 K, melting point of NH_4NO_3; ΔH° = 1.400 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-305.38 K: $Cp^\circ = 36.950 - 12.438\times10^{-3}T$
$H^\circ - H^\circ_{298} = 36.950\times10^{-3}T - 6.219\times10^{-6}T^2 - 10.464$
305.38-357.25 K: $Cp^\circ = 10.112 + 55.402\times10^{-3}T + 1.396\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.112\times10^{-3}T + 27.701\times10^{-6}T^2 - 1.396\times10^{2}T^{-1} - 4.568$
357.25-399 K: $Cp^\circ = -86.341 + 226.158\times10^{-3}T + 52.014\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = -86.341\times10^{-3}T + 113.079\times10^{-6}T^2 - 52.014\times10^{2}T^{-1} + 33.484$
399-442.85 K: $Cp^\circ = 38.477 + 11.080\times10^{-3}T - 7.605\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 38.477\times10^{-3}T + 5.540\times10^{-6}T^2 + 7.605\times10^{2}T^{-1} - 13.080$
442.85-900 K: $Cp^\circ = 38.480$
$H^\circ - H^\circ_{298} = 38.480\times10^{-3}T - 8.878$

Formation equations (kcal/mol):

298.15-305.38 K: $\Delta Hf^\circ = -88.533 + 6.676\times10^{-3}T - 8.401\times10^{-6}T^2 - 26.900T^{-1}$
$\Delta Gf^\circ = -88.533 - 6.676\times10^{-3}T\ln T + 8.401\times10^{-6}T^2 - 13.450T^{-1} + 185.200\times10^{-3}T$
305.38-357.25 K: $\Delta Hf^\circ = -82.638 - 20.162\times10^{-3}T + 25.520\times10^{-6}T^2 - 166.500T^{-1}$
$\Delta Gf^\circ = -82.638 + 20.162\times10^{-3}T\ln T - 25.520\times10^{-6}T^2 - 83.250T^{-1} + 23.446\times10^{-3}T$
357.25-399 K: $\Delta Hf^\circ = -44.586 - 116.615\times10^{-3}T + 110.897\times10^{-6}T^2 - 5228.300T^{-1}$
$\Delta Gf^\circ = -44.586 + 116.615\times10^{-3}T\ln T - 110.897\times10^{-6}T^2 - 2614.150T^{-1} - 599.729\times10^{-3}T$
399-442.85 K: $\Delta Hf^\circ = -91.150 + 8.203\times10^{-3}T + 3.358\times10^{-6}T^2 + 733.600T^{-1}$
$\Delta Gf^\circ = -91.150 - 8.203\times10^{-3}T\ln T - 3.358\times10^{-6}T^2 + 366.800T^{-1} + 202.871\times10^{-3}T$
442.85-900 K: $\Delta Hf^\circ = -86.948 + 8.206\times10^{-3}T - 2.182\times10^{-6}T^2 - 26.900T^{-1}$
$\Delta Gf^\circ = -86.948 - 8.206\times10^{-3}T\ln T + 2.182\times10^{-6}T^2 - 13.450T^{-1} + 192.885\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cox (105). Other data from Gurvich (194).

$(NH_4)_2SO_4(c)$
Ammonium Sulfate
[Reaction: $N_2(g) + 4H_2(g) + 0.5S_2(g) + 2O_2(g) = (NH_4)_2SO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	44.812	52.710	52.710	0	-298.015	-225.520	165.308
300	44.936	52.988	52.711	.083	-298.030	-225.070	163.961
400	51.397	66.804	54.552	4.901	-298.504	-200.662	109.635
500	58.173	78.988	58.240	10.374	-298.406	-176.201	77.016
600	65.745	90.250	62.647	16.562	-297.664	-151.819	55.299
650	69.886	95.674	64.979	19.952	-297.026	-139.690	46.967

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-650 K: $Cp° = 19.699 + 75.560\times10^{-3}T + 2.297\times10^{5}T^{-2}$

$H°-H°_{298} = 19.699\times10^{-3}T + 37.780\times10^{-6}T^2 - 2.297\times10^{2}T^{-1} - 8.461$

Reaction equations (kcal/mol):

298.15-650 K: $\Delta Hr° = -290.804 - 31.274\times10^{-3}T + 34.349\times10^{-6}T^2 - 280.350T^{-1}$

$\Delta Gr° = -290.804 + 31.274\times10^{-3}T\ln T - 34.349\times10^{-6}T^2 - 140.175T^{-1} + 52.599\times10^{-3}T$

Source: Data from DeKock (113).

NOBr(g)
Nitrosyl Bromide (ideal gas)
[Formation: $0.5N_2(g) + 0.5O_2(g) + 0.5Br_2(l,g) = NOBr(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	10.868	65.347	65.347	0	19.630	19.699	-14.439
300	10.879	65.414	65.347	.020	19.621	19.699	-14.351
332.6	11.043	66.545	65.410	.377	19.455	19.716	-12.955
332.6	11.043	66.545	65.410	.377	15.923	19.716	-12.955
400	11.382	68.617	65.779	1.135	15.911	20.485	-11.192
500	11.774	71.200	66.614	2.293	15.911	21.629	-9.454
600	12.107	73.377	67.564	3.488	15.928	22.772	-8.294
700	12.388	75.265	68.532	4.713	15.954	23.910	-7.465
800	12.621	76.935	69.481	5.963	15.986	25.044	-6.842
900	12.813	78.433	70.394	7.235	16.022	26.174	-6.356
1000	12.970	79.791	71.266	8.525	16.061	27.300	-5.966
1100	13.098	81.034	72.099	9.828	16.100	28.421	-5.647
1200	13.204	82.178	72.891	11.144	16.140	29.541	-5.380
1300	13.292	83.239	73.647	12.469	16.179	30.656	-5.154
1400	13.365	84.226	74.367	13.802	16.216	31.769	-4.959
1500	13.427	85.151	75.057	15.141	16.252	32.876	-4.790
1600	13.479	86.019	75.715	16.487	16.287	33.985	-4.642
1700	13.524	86.838	76.346	17.837	16.319	35.088	-4.511
1800	13.562	87.612	76.950	19.191	16.350	36.192	-4.394
1900	13.594	88.346	77.531	20.549	16.378	37.295	-4.290
2000	13.623	89.044	78.089	21.910	16.404	38.394	-4.195

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.756 + 1.170\times10^{-3}T - 1.099\times10^{5}T^{-2}$
$H° - H°_{298} = 11.756\times10^{-3}T + 0.585\times10^{-6}T^{2} + 1.099\times10^{2}T^{-1} - 3.926$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = 20.557 - 4.163\times10^{-3}T + 0.089\times10^{-6}T^{2} + 91.250T^{-1}$
$\Delta Gf° = 20.557 + 4.163\times10^{-3}T\ln T - 0.089\times10^{-6}T^{2} + 45.625T^{-1} - 27.086\times10^{-3}T$
332.6-2000 K: $\Delta Hf° = 15.557 + 0.417\times10^{-3}T + 0.011\times10^{-6}T^{2} + 75.550T^{-1}$
$\Delta Gf° = 15.557 - 0.417\times10^{-3}T\ln T - 0.011\times10^{-6}T^{2} + 37.775T^{-1} + 14.592\times10^{-3}T$

Source: Data from JANAF (127).

NOCl(g)
Nitrosyl Chloride (ideal gas)
[Formation: $0.5N_2(g) + 0.5O_2(g) + 0.5Cl_2(g) = NOCl(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	10.657	62.517	62.517	0	12.360	15.793	-11.577
300	10.670	62.583	62.517	.020	12.359	15.815	-11.521
400	11.269	65.739	62.944	1.118	12.339	16.970	-9.272
500	11.730	68.305	63.767	2.269	12.346	18.128	-7.924
600	12.114	70.479	64.709	3.462	12.371	19.282	-7.023
700	12.437	72.371	65.671	4.690	12.407	20.432	-6.379
800	12.707	74.050	66.616	5.947	12.451	21.573	-5.894
900	12.932	75.560	67.527	7.230	12.502	22.712	-5.515
1000	13.119	76.932	68.400	8.532	12.556	23.843	-5.211
1100	13.278	78.190	69.233	9.853	12.615	24.970	-4.961
1200	13.412	79.352	70.029	11.187	12.676	26.089	-4.751
1300	13.528	80.430	70.788	12.534	12.738	27.204	-4.573
1400	13.630	81.436	71.513	13.892	12.802	28.315	-4.420
1500	13.719	82.380	72.207	15.260	12.867	29.420	-4.286
1600	13.799	83.268	72.870	16.636	12.932	30.521	-4.169
1700	13.871	84.106	73.507	18.019	12.998	31.620	-4.065
1800	13.937	84.901	74.118	19.410	13.066	32.714	-3.972
1900	13.998	85.656	74.705	20.806	13.132	33.804	-3.888
2000	14.054	86.376	75.271	22.209	13.200	34.889	-3.812

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.635 + 1.452 \times 10^{-3}T - 1.254 \times 10^{5}T^{-2}$

$H° - H°_{298} = 11.635 \times 10^{-3}T + 0.726 \times 10^{-6}T^2 + 1.254 \times 10^{2}T^{-1} - 3.954$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 12.001 + 0.348 \times 10^{-3}T + 0.136 \times 10^{-6}T^2 + 72.600T^{-1}$

$\Delta Gf° = 12.001 - 0.348 \times 10^{-3}T\ln T - 0.136 \times 10^{-6}T^2 + 36.300T^{-1} + 14.336 \times 10^{-3}T$

Source: Data from Chase (83).

$NO_2Cl(g)$
Nitryl Chloride (ideal gas)
[Formation: $0.5N_2(g) + O_2(g) + 0.5Cl_2(g) = NO_2Cl(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	12.712	65.030	65.030	0	2.900	12.890	-9.448
300	12.744	65.108	65.030	.024	2.897	12.952	-9.436
400	14.524	68.991	65.549	1.377	2.776	16.325	-8.919
500	15.408	72.302	66.576	2.863	2.753	19.717	-8.618
600	16.291	75.193	67.776	4.450	2.794	23.106	-8.416
700	16.966	77.757	69.023	6.114	2.878	26.486	-8.269
800	17.485	80.058	70.260	7.838	2.989	29.850	-8.154
900	17.886	82.141	71.467	9.607	3.120	33.200	-8.062
1000	18.200	84.043	72.631	11.412	3.264	36.534	-7.984
1100	18.448	85.790	73.749	13.245	3.415	39.854	-7.918
1200	18.648	87.404	74.821	15.100	3.572	43.159	-7.860
1300	18.809	88.903	75.847	16.973	3.733	46.452	-7.809
1400	18.942	90.302	76.830	18.861	3.894	49.732	-7.763
1500	19.052	91.613	77.772	20.761	4.056	53.000	-7.722
1600	19.144	92.845	78.676	22.671	4.217	56.258	-7.684
1700	19.222	94.008	79.544	24.589	4.377	59.507	-7.650
1800	19.288	95.109	80.378	26.515	4.536	62.745	-7.618
1900	19.345	96.153	81.181	28.446	4.690	65.975	-7.589
2000	19.394	97.147	81.956	30.383	4.842	69.195	-7.561

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.033 + 2.172\times10^{-3}T - 3.528\times10^{5}T^{-2}$

$H° - H°_{298} = 16.033\times10^{-3}T + 1.086\times10^{-6}T^{2} + 3.528\times10^{2}T^{-1} - 6.060$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 1.611 + 1.131\times10^{-3}T + 0.245\times10^{-6}T^{2} + 277.400T^{-1}$

$\Delta Gf° = 1.611 - 1.131\times10^{-3}T\ln T - 0.245\times10^{-6}T^{2} + 138.700T^{-1} + 42.786\times10^{-3}T$

Source: Data from JANAF (127).

NOF(g)
Nitrosyl Fluoride (ideal gas)
[Formation: $0.5N_2(g) + 0.5O_2(g) + 0.5F_2(g) = NOF(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	9.883	59.273	59.273	0	-15.700	-12.022	8.812
300	9.899	59.335	59.275	.018	-15.702	-12.000	8.742
400	10.654	62.291	59.671	1.048	-15.760	-10.755	5.876
500	11.229	64.733	60.447	2.143	-15.784	-9.500	4.153
600	11.686	66.822	61.339	3.290	-15.786	-8.243	3.003
700	12.055	68.652	62.256	4.477	-15.776	-6.987	2.181
800	12.352	70.282	63.159	5.698	-15.756	-5.734	1.566
900	12.591	71.751	64.033	6.946	-15.730	-4.481	1.088
1000	12.788	73.086	64.871	8.215	-15.702	-3.231	.706
1100	12.941	74.314	65.677	9.501	-15.672	-1.988	.395
1200	13.069	75.446	66.444	10.802	-15.641	-.745	.136
1300	13.175	76.496	67.178	12.114	-15.610	.496	-.083
1400	13.263	77.476	67.878	13.437	-15.580	1.733	-.271
1500	13.337	78.394	68.549	14.767	-15.550	2.968	-.432
1600	13.399	79.256	69.192	16.103	-15.524	4.202	-.574
1700	13.452	80.070	69.808	17.446	-15.498	5.435	-.699
1800	13.498	80.840	70.399	18.794	-15.474	6.667	-.809
1900	13.537	81.571	70.968	20.145	-15.453	7.895	-.908
2000	13.571	82.267	71.517	21.501	-15.434	9.122	-.997

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.242 + 1.498\times10^{-3}T - 1.605\times10^{5}T^{-2}$

$H°-H°_{298} = 11.242\times10^{-3}T + 0.749\times10^{-6}T^{2} + 1.605\times10^{2}T^{-1} - 3.957$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -16.052 + 0.114\times10^{-3}T + 0.116\times10^{-6}T^{2} + 91.600T^{-1}$

$\Delta Gf° = -16.052 - 0.114\times10^{-3}T\ln T - 0.116\times10^{-6}T^{2} + 45.800T^{-1} + 13.687\times10^{-3}T$

Source: Data from JANAF (127).

$NOF_3(g)$
Trifluoroamine Oxide (ideal gas)
[Formation: $0.5N_2(g) + 0.5O_2(g) + 1.5F_2(g) = NOF_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	16.219	66.535	66.535	0	-39.000	-23.044	16.891
300	16.277	66.636	66.536	.030	-39.004	-22.945	16.716
400	18.824	71.692	67.207	1.794	-39.097	-17.572	9.601
500	20.535	76.089	68.555	3.767	-39.047	-12.195	5.330
600	21.721	79.944	70.139	5.883	-38.910	-6.837	2.490
700	22.569	83.359	71.788	8.100	-38.717	-1.505	.470
800	23.191	86.416	73.428	10.390	-38.491	3.794	-1.036
900	23.658	89.175	75.027	12.733	-38.241	9.067	-2.202
1000	24.016	91.687	76.569	15.118	-37.977	14.308	-3.127
1100	24.295	93.990	78.050	17.534	-37.704	19.523	-3.879
1200	24.517	96.114	79.468	19.975	-37.423	24.713	-4.501
1300	24.695	98.083	80.825	22.436	-37.138	29.882	-5.024
1400	24.840	99.919	82.124	24.913	-36.854	35.024	-5.467
1500	24.959	101.637	83.368	27.403	-36.568	40.148	-5.849
1600	25.059	103.251	84.561	29.904	-36.282	45.253	-6.181
1700	25.142	104.773	85.706	32.414	-35.996	50.341	-6.472
1800	25.213	106.212	86.805	34.932	-35.715	55.412	-6.728
1900	25.274	107.577	87.863	37.456	-35.433	60.467	-6.955
2000	25.326	108.875	88.882	39.986	-35.158	65.506	-7.158

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 22.092 + 2.140\text{x}10^{-3}T - 5.788\text{x}10^{5}T^{-2}$

$H° - H°_{298} = 22.092\text{x}10^{-3}T + 1.070\text{x}10^{-6}T^{2} + 5.788\text{x}10^{2}T^{-1} - 8.623$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -41.129 + 2.456\text{x}10^{-3}T + 0.263\text{x}10^{-6}T^{2} + 409.400T^{-1}$

$\Delta Gf° = -41.129 - 2.456\text{x}10^{-3}T\ln T - 0.263\text{x}10^{-6}T^{2} + 204.700T^{-1} + 72.429\text{x}10^{-3}T$

Source: Data from JANAF (127) who estimated some molecular constants.

$NO_2F(g)$
Nitryl Fluoride (ideal gas)
[Formation: $0.5N_2(g) + O_2(g) + 0.5F_2(g) = NO_2F(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.918	62.177	62.177	0	-26.000	-15.882	11.642
300	11.953	62.251	62.178	.022	-26.005	-15.820	11.525
400	13.626	65.929	62.667	1.305	-26.164	-12.397	6.773
500	14.903	69.114	63.646	2.734	-26.220	-8.947	3.911
600	15.876	71.921	64.796	4.275	-26.206	-5.493	2.001
700	16.620	74.426	65.995	5.902	-26.144	-2.044	.638
800	17.193	76.685	67.192	7.594	-26.052	1.392	-.380
900	17.638	78.737	68.364	9.336	-25.940	4.816	-1.169
1000	17.987	80.614	69.496	11.118	-25.812	8.226	-1.798
1100	18.265	82.342	70.587	12.931	-25.675	11.623	-2.309
1200	18.488	83.941	71.633	14.769	-25.531	15.008	-2.733
1300	18.669	85.428	72.638	16.627	-25.381	18.381	-3.090
1400	18.819	86.817	73.601	18.502	-25.231	21.741	-3.394
1500	18.942	88.120	74.527	20.390	-25.079	25.090	-3.656
1600	19.046	89.346	75.415	22.290	-24.927	28.430	-3.883
1700	19.134	90.503	76.268	24.199	-24.776	31.761	-4.083
1800	19.209	91.599	77.090	26.116	-24.627	35.083	-4.260
1900	19.273	92.639	77.881	28.040	-24.479	38.396	-4.417
2000	19.328	93.629	78.644	29.970	-24.336	41.701	-4.557

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 15.326 + 2.628x10^{-3}T - 3.726x10^{5}T^{-2}$

$H°- H°_{298} = 15.326x10^{-3}T + 1.314x10^{-6}T^{2} + 3.726x10^{2}T^{-1} - 5.936$

Formation equations (kcal/mol):

298.15-2000 K: $ΔHf° = -27.155 + 0.583x10^{-3}T + 0.430x10^{-6}T^{2} + 281.100T^{-1}$

$ΔGf° = -27.155 - 0.583x10^{-3}T\ln T - 0.430x10^{-6}T^{2} + 140.550T^{-1} + 39.680x10^{-3}T$

Source: Data from JANAF (127).

NOI(g)
Nitrosyl Iodide (ideal gas)

[Formation: $0.5N_2(g) + 0.5O_2(g) + 0.5I_2(c,l,g) = NOI(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.199	67.581	67.581	0	26.800	24.917	-18.265
300	11.208	67.650	67.581	.021	26.796	24.906	-18.144
386.8	11.554	70.543	67.934	1.009	26.570	24.387	-13.779
386.8	11.554	70.543	67.934	1.009	24.716	24.387	-13.779
400	11.607	70.932	68.027	1.162	24.647	24.377	-13.319
458.4	11.800	72.528	68.500	1.846	24.353	24.359	-11.613
458.4	11.800	72.528	68.500	1.846	19.342	24.359	-11.613
500	11.938	73.559	68.879	2.340	19.349	24.815	-10.846
600	12.232	75.762	69.847	3.549	19.376	25.906	-9.436
700	12.487	77.667	70.831	4.785	19.410	26.991	-8.427
800	12.702	79.349	71.793	6.045	19.449	28.072	-7.669
900	12.880	80.856	72.718	7.324	19.490	29.147	-7.078
1000	13.026	82.220	73.600	8.620	19.532	30.218	-6.604
1100	13.147	83.468	74.442	9.929	19.574	31.285	-6.216
1200	13.246	84.616	75.242	11.249	19.615	32.348	-5.891
1300	13.328	85.680	76.005	12.577	19.655	33.407	-5.616
1400	13.397	86.670	76.731	13.914	19.694	34.464	-5.380
1500	13.455	87.596	77.425	15.257	19.731	35.518	-5.175
1600	13.504	88.466	78.088	16.605	19.765	36.570	-4.995
1700	13.546	89.286	78.723	17.957	19.797	37.618	-4.836
1800	13.582	90.062	79.332	19.314	19.827	38.665	-4.695
1900	13.613	90.797	79.916	20.673	19.853	39.710	-4.568
2000	13.640	91.496	80.478	22.036	19.878	40.755	-4.453

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.848 + 1.120\times10^{-3}T - 0.874\times10^{5}T^{-2}$
$H°- H°_{298} = 11.848\times10^{-3}T + 0.560\times10^{-6}T^{2} + 0.874\times10^{2}T^{-1} - 3.875$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = 27.071 - 1.464\times10^{-3}T - 0.732\times10^{-6}T^{2} + 68.750T^{-1}$
$\Delta Gf° = 27.071 + 1.464\times10^{-3}T\ln T + 0.732\times10^{-6}T^{2} + 34.375T^{-1} - 16.170\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = 26.343 - 4.666\times10^{-3}T + 0.014\times10^{-6}T^{2} + 68.750T^{-1}$
$\Delta Gf° = 26.343 + 4.666\times10^{-3}T\ln T - 0.014\times10^{-6}T^{2} + 34.375T^{-1} - 33.077\times10^{-3}T$
458.4-2000 K: $\Delta Hf° = 18.987 + 0.504\times10^{-3}T - 0.020\times10^{-6}T^{2} + 61.100T^{-1}$
$\Delta Gf° = 18.987 - 0.504\times10^{-3}T\ln T + 0.020\times10^{-6}T^{2} + 30.550T^{-1} + 14.654\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$NaAlCO_3(OH)_2$(dawsonite)
Dawsonite

[Formation: $Na(c,l) + Al(c) + C(c) + H_2(g) + 2.5O_2(g) = NaAlCO_3(OH)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	34.081	31.555	31.555	0	-469.400	-426.881	312.908
300	34.221	31.766	31.556	.063	-469.410	-426.616	310.786
325	35.981	34.574	31.682	.940	-469.517	-423.046	284.478
350	37.701	37.304	31.984	1.862	-469.594	-419.468	261.924
371	39.153	39.543	32.349	2.669	-469.641	-416.459	245.326
371	39.153	39.543	32.349	2.669	-470.263	-416.459	245.326
375	39.430	39.964	32.428	2.826	-470.270	-415.879	242.371
400	41.223	42.565	32.980	3.834	-470.293	-412.251	225.241
425	43.118	45.121	33.620	4.888	-470.280	-408.624	210.126
450	45.145	47.642	34.329	5.991	-470.224	-404.998	196.691
475	47.325	50.140	35.096	7.146	-470.125	-401.377	184.673
477	47.507	50.340	35.160	7.241	-470.115	-401.087	183.766

Phase change: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-477 K: $Cp° = 8.223 + 79.994\times10^{-3}T + 1.784\times10^{5}T^{-2}$
$H°- H°_{298} = 8.223\times10^{-3}T + 39.997\times10^{-6}T^{2} - 1.784\times10^{2}T^{-1} - 5.409$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -462.271 - 28.369\times10^{-3}T + 31.170\times10^{-6}T^{2} - 429.800T^{-1}$
$\Delta Gf° = -462.271 + 28.369\times10^{-3}T\ln T - 31.170\times10^{-6}T^{2} - 214.900T^{-1} - 31.225\times10^{-3}T$
371-477 K: $\Delta Hf° = -462.659 - 31.422\times10^{-3}T + 35.919\times10^{-6}T^{2} - 338.900T^{-1}$
$\Delta Gf° = -462.659 + 31.422\times10^{-3}T\ln T - 35.919\times10^{-6}T^{2} - 169.450T^{-1} - 46.809\times10^{-3}T$

Source: Data from Ferrante (148).

$NaAlCl_4(c,l)$
Sodium Tetrachloroaluminate
[Formation: $Na(c,l) + Al(c,l) + 2Cl_2(g) = NaAlCl_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	31.550	47.600	47.600	0	-272.300	-249.028	182.540
300	31.669	47.796	47.603	.058	-272.295	-248.884	181.310
371	34.596	54.907	48.329	2.440	-272.011	-243.372	143.364
371	34.596	54.907	48.329	2.440	-272.633	-243.372	143.364
400	35.792	57.556	48.903	3.461	-272.494	-241.090	131.724
426	36.420	59.830	49.502	4.400	-272.350	-239.053	122.639
426	42.000	70.605	49.502	8.990	-267.760	-239.053	122.639
500	42.000	77.332	53.136	12.098	-266.928	-234.134	102.338
600	42.000	84.989	57.826	16.298	-265.838	-227.676	82.930
700	42.000	91.464	62.181	20.498	-264.782	-221.402	69.124
800	42.000	97.072	66.200	24.698	-263.768	-215.275	58.810
900	42.000	102.019	69.910	28.898	-262.798	-209.271	50.817
933.61	42.000	103.559	71.094	30.310	-262.483	-207.278	48.521
933.61	42.000	103.559	71.094	30.310	-265.063	-207.278	48.521
1000	42.000	106.444	73.346	33.098	-264.426	-203.193	44.407

*Heat capacity at 298 K estimated and data extrapolated above 573 K.

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
426 K, melting point of $NaAlCl_4$; ΔH° = 4.590 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-426 K:
$Cp° = 41.094 - 8.482\times10^{5}T^{-2}$
$H°-H°_{298} = 41.094\times10^{-3}T + 8.482\times10^{2}T^{-1} - 15.097$

426-1000 K:
$Cp° = 42.000$
$H°-H°_{298} = 42.000\times10^{-3}T - 8.902$

Formation equations (kcal/mol):

298.15-371 K:
$\Delta Hf° = -278.603 + 14.897\times10^{-3}T - 6.561\times10^{-6}T^{2} + 729.000T^{-1}$
$\Delta Gf° = -278.603 - 14.897\times10^{-3}T\ln T + 6.561\times10^{-6}T^{2} + 364.500T^{-1} + 178.016\times10^{-3}T$

371-426 K:
$\Delta Hf° = -278.992 + 11.844\times10^{-3}T - 1.811\times10^{-6}T^{2} + 819.900T^{-1}$
$\Delta Gf° = -278.992 - 11.844\times10^{-3}T\ln T + 1.811\times10^{-6}T^{2} + 409.950T^{-1} + 162.432\times10^{-3}T$

426-933.61 K:
$\Delta Hf° = -272.796 + 12.750\times10^{-3}T - 1.811\times10^{-6}T^{2} - 28.300T^{-1}$
$\Delta Gf° = -272.796 - 12.750\times10^{-3}T\ln T + 1.811\times10^{-6}T^{2} - 14.150T^{-1} + 155.712\times10^{-3}T$

933.61-1000 K:
$\Delta Hf° = -274.064 + 9.752\times10^{-3}T - 0.084\times10^{-6}T^{2} - 45.700T^{-1}$
$\Delta Gf° = -274.064 - 9.752\times10^{-3}T\ln T + 0.084\times10^{-6}T^{2} - 22.850T^{-1} + 138.189\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Rogers (430). Entropy at 298 K from Dewing (122). Heat capacity at 298 K estimated. High-temperature data based on Rogers (430). Data extrapolated above 573 K.

$NaAlF_4(g)$
Sodium Tetrafluoroaluminate (ideal gas)
[Formation: $Na(c,l,g) + Al(c,l) + 2F_2(g) = NaAlF_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.846	82.406	82.406	0	-440.000	-429.996	315.191
300	24.900	82.560	82.407	.046	-440.005	-429.934	313.203
371	26.518	88.043	82.972	1.881	-440.178	-427.530	251.848
371	26.518	88.043	82.972	1.881	-440.800	-427.530	251.848
400	27.179	90.064	83.414	2.660	-440.871	-426.490	233.020
500	28.553	96.288	85.384	5.452	-441.052	-422.872	184.835
600	29.417	101.576	87.653	8.354	-441.182	-419.222	152.700
700	29.987	106.157	89.977	11.326	-441.294	-415.554	129.740
800	30.378	110.188	92.257	14.345	-441.413	-411.871	112.516
900	30.657	113.783	94.452	17.398	-441.552	-408.167	99.115
933.61	30.726	114.908	95.168	18.430	-441.607	-406.920	95.255
933.61	30.726	114.908	95.168	18.430	-444.187	-406.920	95.255
1000	30.863	117.024	96.550	20.474	-444.276	-404.269	88.352
1100	31.018	119.973	98.548	23.568	-444.409	-400.263	79.524
1177	31.110	122.075	100.018	25.960	-444.513	-397.164	73.746
1177	31.110	122.075	100.018	25.960	-467.798	-397.164	73.746
1200	31.137	122.677	100.447	26.676	-467.783	-395.787	72.082
1300	31.232	125.174	102.255	29.795	-467.709	-389.787	65.528
1400	31.307	127.491	103.975	32.922	-467.638	-383.798	59.913
1500	31.369	129.653	105.616	36.056	-467.566	-377.813	55.047
1600	31.419	131.679	107.182	39.196	-467.494	-371.830	50.789
1700	31.461	133.585	108.679	42.340	-467.422	-365.852	47.033
1800	31.497	135.385	110.114	45.488	-467.354	-359.881	43.695
1900	31.527	137.089	111.490	48.639	-467.285	-353.910	40.708
2000	31.553	138.706	112.809	51.793	-467.221	-347.945	38.021

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 30.173 + 0.998\times10^{-3}T - 5.000\times10^{5}T^{-2}$
$H°- H°_{298} = 30.173\times10^{-3}T + 0.499\times10^{-6}T^{2} + 5.000\times10^{2}T^{-1} - 10.717$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -441.883 + 4.614\times10^{-3}T - 6.234\times10^{-6}T^{2} + 316.400T^{-1}$
$\Delta Gf° = -441.883 - 4.614\times10^{-3}T\ln T + 6.234\times10^{-6}T^{2} + 158.200T^{-1} + 62.519\times10^{-3}T$
371-933.61 K: $\Delta Hf° = -442.271 + 1.561\times10^{-3}T - 1.484\times10^{-6}T^{2} + 407.300T^{-1}$
$\Delta Gf° = -442.271 - 1.561\times10^{-3}T\ln T + 1.484\times10^{-6}T^{2} + 203.650T^{-1} + 46.935\times10^{-3}T$
933.61-1177 K: $\Delta Hf° = -443.539 - 1.437\times10^{-3}T + 0.243\times10^{-6}T^{2} + 389.900T^{-1}$
$\Delta Gf° = -443.539 + 1.437\times10^{-3}T\ln T - 0.243\times10^{-6}T^{2} + 194.950T^{-1} + 29.412\times10^{-3}T$
1177-2000 K: $\Delta Hf° = -469.002 + 0.600\times10^{-3}T + 0.147\times10^{-6}T^{2} + 288.000T^{-1}$
$\Delta Gf° = -469.002 - 0.600\times10^{-3}T\ln T - 0.147\times10^{-6}T^{2} + 144.000T^{-1} + 65.372\times10^{-3}T$

Source: Data from JANAF (131).

Na_3AlF_6(c,l)
Trisodium Aluminum Hexafluoride, Cryolite
[Formation: $3Na(c,l,g) + Al(c,l) + 3F_2(g) = Na_3AlF_6(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	51.560	56.995	56.995	0	-792.760	-753.403	552.252
300	51.676	57.314	56.997	.095	-792.754	-753.159	548.669
371	55.098	68.699	58.171	3.906	-792.500	-743.814	438.163
371	55.098	68.699	58.171	3.906	-794.366	-743.814	438.163
400	56.496	72.898	59.088	5.524	-794.262	-739.866	404.239
500	59.425	85.787	63.175	11.306	-793.739	-726.321	317.470
600	62.809	96.921	67.891	17.418	-792.931	-712.908	259.673
700	66.162	106.855	72.759	23.867	-791.826	-699.656	218.440
800	69.498	115.908	77.595	30.650	-790.433	-686.582	187.563
836	70.700	118.993	79.313	33.173	-789.863	-681.921	178.268
836	62.500	121.697	79.313	35.433	-787.603	-681.921	178.268
900	64.880	126.394	82.495	39.509	-787.017	-673.849	163.631
933.61	66.140	128.796	84.119	41.711	-786.660	-669.630	156.752
933.61	66.140	128.796	84.119	41.711	-789.240	-669.630	156.752
1000	68.630	133.423	87.239	46.184	-788.402	-661.155	144.493
1100	72.410	140.142	91.746	53.236	-786.855	-648.506	128.845
1177	75.336	145.139	95.076	58.924	-785.428	-638.856	118.624
1177	75.336	145.139	95.076	58.924	-855.283	-638.856	118.624
1200	76.210	146.605	96.049	60.667	-854.679	-634.640	115.582
1285	79.460	151.930	99.570	67.283	-852.254	-619.126	105.298
1285	94.530	172.397	99.570	93.583	-825.954	-619.126	105.298
1300	94.530	173.494	100.416	95.001	-825.277	-616.715	103.678
1400*	94.530	180.500	105.890	104.454	-820.774	-600.847	93.795
1500	94.530	187.022	111.084	113.907	-816.280	-585.300	85.277
1600	94.530	193.123	116.023	123.360	-811.795	-570.045	77.863
1700	94.530	198.853	120.728	132.813	-807.316	-555.070	71.358
1800	94.530	204.257	125.220	142.266	-802.849	-540.364	65.608
1900	94.530	209.368	129.516	151.719	-798.385	-525.898	60.491
2000	94.530	214.216	133.630	161.172	-793.933	-511.673	55.912

*Data extrapolated above 1370 K.

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
836 K, α - β transition point of Na_3AlF_6; ΔH° = 2.260 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1285 K, melting point of Na_3AlF_6; ΔH° = 26.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-836 K: $Cp° = 47.260 + 27.962x10^{-3}T - 3.589x10^{5}T^{-2}$
$H°- H°_{298} = 47.260x10^{-3}T + 13.981x10^{-6}T^{2} + 3.589x10^{2}T^{-1} - 16.537$
836-1285 K: $Cp° = 29.490 + 38.654x10^{-3}T + 4.857x10^{5}T^{-2}$
$H°- H°_{298} = 29.490x10^{-3}T + 19.327x10^{-6}T^{2} - 4.857x10^{2}T^{-1} - 2.147$
1285-2000 K: $Cp° = 94.530$
$H°- H°_{298} = 94.530x10^{-3}T - 27.888$

Formation equations (kcal/mol):

298.15-371 K: $ΔHf° = -794.389 + 5.291x10^{-3}T - 2.242x10^{-6}T^{2} + 74.800T^{-1}$
$ΔGf° = -794.389 - 5.291x10^{-3}TlnT + 2.242x10^{-6}T^{2} + 37.400T^{-1} + 166.525x10^{-3}T$
371-836 K: $ΔHf° = -795.554 - 3.868x10^{-3}T + 12.008x10^{-6}T^{2} + 347.500T^{-1}$
$ΔGf° = -795.554 + 3.868x10^{-3}TlnT - 12.008x10^{-6}T^{2} + 173.750T^{-1} + 119.773x10^{-3}T$
836-933.61 K: $ΔHf° = -781.164 - 21.638x10^{-3}T + 17.354x10^{-6}T^{2} - 497.100T^{-1}$
$ΔGf° = -781.164 + 21.638x10^{-3}TlnT - 17.354x10^{-6}T^{2} - 248.550T^{-1} - 11.934x10^{-3}T$
933.61-1177 K: $ΔHf° = -782.432 - 24.636x10^{-3}T + 19.081x10^{-6}T^{2} - 514.500T^{-1}$
$ΔGf° = -782.432 + 24.636x10^{-3}TlnT - 19.081x10^{-6}T^{2} - 257.250T^{-1} - 29.457x10^{-3}T$
1177-1285 K: $ΔHf° = -858.821 - 18.525x10^{-3}T + 18.793x10^{-6}T^{2} - 820.200T^{-1}$
$ΔGf° = -858.821 + 18.525x10^{-3}TlnT - 18.793x10^{-6}T^{2} - 410.100T^{-1} + 78.425x10^{-3}T$
1285-2000 K: $ΔHf° = -884.562 + 46.515x10^{-3}T - 0.534x10^{-6}T^{2} - 334.500T^{-1}$
$ΔGf° = -884.562 - 46.515x10^{-3}TlnT + 0.534x10^{-6}T^{2} - 167.250T^{-1} + 539.064x10^{-3}T$

Source: Data from JANAF (131) who extrapolated above 1370 K.

$Na_5Al_3F_{14}$(c)
Sodium Aluminum Fluoride, Chiolite
[Formation: $5Na(c,l) + 3Al(c,l) + 7F_2(g) = Na_5Al_3F_{14}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	108.490	123.146	123.146	0	-1803.600	-1714.819	1256.980
300	108.760	123.818	123.148	.201	-1803.590	-1714.268	1248.827
371	116.321	147.871	125.626	8.253	-1803.113	-1693.175	997.408
371	116.321	147.871	125.626	8.253	-1806.223	-1693.175	997.408
400	119.409	156.742	127.565	11.671	-1806.017	-1684.346	920.272
500	125.440	184.085	136.213	23.936	-1804.957	-1654.038	722.970
600	129.656	207.346	146.179	36.700	-1803.561	-1623.982	591.527
700	133.016	227.593	156.394	49.839	-1801.934	-1594.182	497.720
800	135.919	245.548	166.438	63.288	-1800.151	-1564.626	427.431
900	138.556	261.711	176.140	77.014	-1798.252	-1535.291	372.815
933.61	139.387	266.806	179.313	81.685	-1797.599	-1525.482	357.097
933.61	139.387	266.806	179.313	81.685	-1805.339	-1525.482	357.097
1000	141.028	276.438	185.444	90.994	-1803.932	-1505.638	329.053
1010	141.269	277.843	186.353	92.405	-1803.713	-1502.657	325.150

Phase changes: 371 K, melting point of Na; $\Delta H° = 0.622$ kcal/mol.
933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1010 K: $Cp° = 122.193 + 20.602\times10^{-3}T - 17.642\times10^{5}T^{-2}$
$H°-H°_{298} = 122.193\times10^{-3}T + 10.301\times10^{-6}T^{2} + 17.642\times10^{2}T^{-1} - 43.265$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -1814.287 + 29.106\times10^{-3}T - 19.388\times10^{-6}T^{2} + 1112.900T^{-1}$
$\Delta Gf° = -1814.287 - 29.106\times10^{-3}T\ln T + 19.388\times10^{-6}T^{2} + 556.450T^{-1} + 487.412\times10^{-3}T$
371-933.61 K: $\Delta Hf° = -1816.228 + 13.841\times10^{-3}T + 4.362\times10^{-6}T^{2} + 1567.400T^{-1}$
$\Delta Gf° = -1816.228 - 13.841\times10^{-3}T\ln T - 4.362\times10^{-6}T^{2} + 783.700T^{-1} + 409.492\times10^{-3}T$
933.61-1010 K: $\Delta Hf° = -1820.031 + 4.847\times10^{-3}T + 9.543\times10^{-6}T^{2} + 1515.200T^{-1}$
$\Delta Gf° = -1820.031 - 4.847\times10^{-3}T\ln T - 9.543\times10^{-6}T^{2} + 757.600T^{-1} + 356.922\times10^{-3}T$

Source: Data from Stuve (482).

$NaAlO_2(c)$
Sodium Aluminate
[Formation: $Na(c,l,g) + Al(c,l) + O_2(g) = NaAlO_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	17.573	16.870	16.870	0	-271.300	-256.032	187.674
300	17.633	16.979	16.870	.033	-271.303	-255.936	186.447
371	19.280	20.927	17.274	1.355	-271.408	-252.287	148.616
371	19.280	20.927	17.274	1.355	-272.030	-252.287	148.616
400	19.953	22.403	17.593	1.924	-272.064	-250.743	136.998
500	21.385	27.019	19.029	3.995	-272.089	-245.406	107.266
600	22.468	31.017	20.702	6.189	-272.022	-240.074	87.446
700	23.387	34.551	22.432	8.483	-271.894	-234.760	73.294
740	23.727	35.860	23.123	9.425	-271.831	-232.640	68.706
740	23.396	36.292	23.123	9.745	-271.511	-232.640	68.706
800	23.643	38.126	24.180	11.157	-271.432	-229.491	62.693
900	24.055	40.935	25.889	13.541	-271.312	-224.257	54.456
933.61	24.194	41.819	26.447	14.352	-271.275	-222.501	52.085
933.61	24.194	41.819	26.447	14.352	-273.855	-222.501	52.085
1000	24.468	43.490	27.522	15.968	-273.752	-218.851	47.829
1100	24.880	45.842	29.083	18.435	-273.579	-213.372	42.392
1177	25.198	47.535	30.234	20.363	-273.427	-209.156	38.836
1177	25.198	47.535	30.234	20.363	-296.712	-209.156	38.836
1200	25.293	48.024	30.571	20.944	-296.618	-207.448	37.781
1300	25.705	50.065	31.993	23.494	-296.179	-200.034	33.628
1400	26.118	51.985	33.353	26.085	-295.708	-192.655	30.074
1500	26.530	53.801	34.656	28.717	-295.202	-185.315	27.000
1600	26.943	55.527	35.908	31.391	-294.661	-178.007	24.314
1700	27.355	57.172	37.110	34.106	-294.084	-170.732	21.949
1800	27.767	58.748	38.269	36.862	-293.472	-163.494	19.851
1900	28.180	60.260	39.387	39.659	-292.825	-156.289	17.977
2000	28.592	61.716	40.467	42.498	-292.141	-149.121	16.295

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
740 K, α – β transition point of $NaAlO_2$; ΔH° = 0.320 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-740 K: $Cp° = 19.405 + 6.680\times10^{-3}T - 3.399\times10^{5}T^{-2}$
$H°-H°_{298} = 19.405\times10^{-3}T + 3.340\times10^{-6}T^{2} + 3.399\times10^{2}T^{-1} - 7.223$
740-2000 K: $Cp° = 20.342 + 4.126\times10^{-3}T$
$H°-H°_{298} = 20.342\times10^{-3}T + 2.063\times10^{-6}T^{2} - 6.438$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -273.114 + 3.632\times10^{-3}T - 3.548\times10^{-6}T^{2} + 312.100T^{-1}$
$\Delta Gf° = -273.114 - 3.632\times10^{-3}T\ln T + 3.548\times10^{-6}T^{2} + 156.050T^{-1} + 75.174\times10^{-3}T$
371-740 K: $\Delta Hf° = -273.502 + 0.579\times10^{-3}T + 1.202\times10^{-6}T^{2} + 403.000T^{-1}$
$\Delta Gf° = -273.502 - 0.579\times10^{-3}T\ln T - 1.202\times10^{-6}T^{2} + 201.500T^{-1} + 59.590\times10^{-3}T$
740-933.61 K: $\Delta Hf° = -272.717 + 1.516\times10^{-3}T - 0.075\times10^{-6}T^{2} + 63.100T^{-1}$
$\Delta Gf° = -272.717 - 1.516\times10^{-3}T\ln T + 0.075\times10^{-6}T^{2} + 31.550T^{-1} + 64.085\times10^{-3}T$
933.61-1177 K: $\Delta Hf° = -273.985 - 1.482\times10^{-3}T + 1.652\times10^{-6}T^{2} + 45.700T^{-1}$
$\Delta Gf° = -273.985 + 1.482\times10^{-3}T\ln T - 1.652\times10^{-6}T^{2} + 22.850T^{-1} + 46.562\times10^{-3}T$
1177-2000 K: $\Delta Hf° = -299.448 + 0.555\times10^{-3}T + 1.556\times10^{-6}T^{2} - 56.200T^{-1}$
$\Delta Gf° = -299.448 - 0.555\times10^{-3}T\ln T - 1.556\times10^{-6}T^{2} - 28.100T^{-1} + 82.522\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from King (260). High-temperature data based on Christensen (93).

$NaAlSiO_4$(nepheline)
Sodium Aluminum Silicate, Nepheline
[Formation: $Na(c,l,g) + Al(c,l) + Si(c) + 2O_2(g) = NaAlSiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	28.400	29.700	29.700	0	-500.300	-472.905	346.644
300	28.504	29.876	29.700	.053	-500.305	-472.734	344.382
371	32.310	36.301	30.359	2.204	-500.438	-466.195	274.624
371	32.310	36.301	30.359	2.204	-501.060	-466.195	274.624
400	33.864	38.791	30.881	3.164	-501.063	-463.469	253.224
467	41.868	44.546	32.426	5.660	-500.817	-457.183	213.953
467	36.302	44.546	32.426	5.660	-500.817	-457.183	213.953
500	36.063	47.015	33.309	6.853	-500.747	-454.102	198.485
600	36.313	53.594	36.157	10.462	-500.592	-444.788	162.012
700	37.419	59.267	39.061	14.144	-500.445	-435.500	135.967
800	38.980	64.362	41.911	17.961	-500.243	-426.235	116.440
900	40.806	69.057	44.669	21.949	-499.953	-417.000	101.260
933.61	41.475	70.565	45.574	23.332	-499.831	-413.904	96.890
933.61	41.475	70.565	45.574	23.332	-502.411	-413.904	96.890
1000	42.797	73.458	47.330	26.128	-502.096	-407.613	89.083
1100	44.896	77.635	49.897	30.512	-501.482	-398.202	79.114
1177	46.566	80.728	51.813	34.033	-500.885	-390.987	72.599
1177	46.566	80.728	51.813	34.033	-524.170	-390.987	72.599
1190	46.848	81.241	52.132	34.640	-524.033	-389.519	71.536
1190	42.624	81.241	52.132	34.640	-524.033	-389.519	71.536
1200	42.636	81.598	52.376	35.066	-523.968	-388.390	70.734
1300	42.759	85.015	54.757	39.336	-523.315	-377.116	63.398
1400	42.882	88.189	57.033	43.618	-522.674	-365.891	57.117
1500	43.005	91.151	59.210	47.912	-522.039	-354.727	51.683
1525	43.035	91.862	59.739	48.988	-521.880	-351.940	50.436

Phase change: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
467 K, second order transition point of $NaAlSiO_4$; ΔH° = 0 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1177 K, boiling poing of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1190 K, second order transition point of $NaAlSiO_4$; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-467 K: $Cp° = -16.087 + 110.318\times10^{-3}T + 10.308\times10^{5}T^{-2}$
$H°-H°_{298} = -16.087\times10^{-3}T + 55.159\times10^{-6}T^2 - 10.308\times10^{2}T^{-1} + 3.350$
467-1190 K: $Cp° = 16.991 + 24.044\times10^{-3}T + 17.628\times10^{5}T^{-2}$
$H°-H°_{298} = 16.991\times10^{-3}T + 12.022\times10^{-6}T^2 - 17.628\times10^{2}T^{-1} - 1.122$
1190-1525 K: $Cp° = 41.281 + 1.164\times10^{-3}T - 0.588\times10^{5}T^{-2}$
$H°-H°_{298} = 41.281\times10^{-3}T + 0.582\times10^{-6}T^2 + 0.588\times10^{2}T^{-1} - 15.358$

Formation equations (kcal/mol):

298.15-371 K: $ΔHf° = -487.135 - 44.769\times10^{-3}T + 47.417\times10^{-6}T^2 - 1202.300T^{-1}$
$ΔGf° = -487.135 + 44.769\times10^{-3}T\ln T - 47.417\times10^{-6}T^2 - 601.150T^{-1} - 186.449\times10^{-3}T$
371-467 K: $ΔHf° = -487.523 - 47.822\times10^{-3}T + 52.167\times10^{-6}T^2 - 1111.400T^{-1}$
$ΔGf° = -487.523 + 47.822\times10^{-3}T\ln T - 52.167\times10^{-6}T^2 - 555.700T^{-1} - 202.032\times10^{-3}T$
467-933.61 K: $ΔHf° = -491.995 - 14.744\times10^{-3}T + 9.030\times10^{-6}T^2 - 1843.400T^{-1}$
$ΔGf° = -491.995 + 14.744\times10^{-3}T\ln T - 9.030\times10^{-6}T^2 - 921.700T^{-1} - 7.614\times10^{-3}T$
933.61-1177 K: $ΔHf° = -493.263 - 17.742\times10^{-3}T + 10.757\times10^{-6}T^2 - 1860.800T^{-1}$
$ΔGf° = -493.263 + 17.742\times10^{-3}T\ln T - 10.757\times10^{-6}T^2 - 930.400T^{-1} - 25.138\times10^{-3}T$
1177-1190 K: $ΔHf° = -518.726 - 15.705\times10^{-3}T + 10.661\times10^{-6}T^2 - 1962.700T^{-1}$
$ΔGf° = -518.726 + 15.705\times10^{-3}T\ln T - 10.661\times10^{-6}T^2 - 981.350T^{-1} + 10.823\times10^{-3}T$
1190-1525 K: $ΔHf° = -532.961 + 8.585\times10^{-3}T - 0.779\times10^{-6}T^2 - 141.100T^{-1}$
$ΔGf° = -532.961 - 8.585\times10^{-3}T\ln T + 0.779\times10^{-6}T^2 - 70.550T^{-1} + 180.544\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Barany (19) and Navrotsky (349). Other data based on Kelley (250) and Henderson (205).

$NaAlSi_2O_6$(jadeite)
Sodium aluminum Disilicate, Jadeite

[Formation: $Na(c,l,g) + Al(c,l) + 2Si(c) + 3O_2(g) = NaAlSi_2O_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	38.230	31.900	31.900	0	-724.400	-681.708	499.699
300	38.400	32.140	31.907	.070	-724.410	-681.444	496.425
371	43.079	40.866	32.798	2.993	-724.629	-671.252	395.418
371	43.079	40.866	32.798	2.993	-725.251	-671.252	395.418
400	44.990	44.180	33.505	4.270	-725.296	-667.030	364.443
500	48.980	54.680	36.700	8.990	-725.226	-652.453	285.183
600	51.840	63.880	40.497	14.030	-724.967	-637.933	232.364
700	54.050	72.040	44.426	19.330	-724.571	-623.455	194.649
800	55.820	79.380	48.342	24.830	-724.089	-609.039	166.380
900	57.250	86.040	52.162	30.490	-723.561	-594.685	144.407
933.61	57.630	88.146	53.420	32.421	-723.378	-589.875	138.083
933.61	57.630	88.146	53.420	32.421	-725.958	-589.875	138.083
1000	58.380	92.130	55.860	36.270	-725.558	-580.197	126.800
1100	59.260	97.740	59.422	42.150	-724.924	-565.714	112.396
1177	59.745	101.762	62.056	46.734	-724.411	-554.576	102.974
1177	59.745	101.762	62.056	46.734	-747.696	-554.576	102.974
1200	59.890	102.920	62.828	48.110	-747.496	-550.806	100.314

Phase changes: 371 K, melting point of Na; $\Delta H° = 0.622$ kcal/mol.
933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; $\Delta H° = 23.285$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 47.426 + 12.346\times10^{-3}T - 11.446\times10^{5}T^{-2}$
$H°-H°_{298} = 47.426\times10^{-3}T + 6.173\times10^{-6}T^{2} + 11.446\times10^{2}T^{-1} - 18.528$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -728.706 + 5.835\times10^{-3}T - 2.423\times10^{-6}T^{2} + 829.400T^{-1}$
$\Delta Gf° = -728.706 - 5.835\times10^{-3}T\ln T + 2.423\times10^{-6}T^{2} + 414.700T^{-1} + 185.490\times10^{-3}T$
371-933.61 K: $\Delta Hf° = -729.094 + 2.782\times10^{-3}T + 2.327\times10^{-6}T^{2} + 920.300T^{-1}$
$\Delta Gf° = -729.094 - 2.782\times10^{-3}T\ln T - 2.327\times10^{-6}T^{2} + 460.150T^{-1} + 169.905\times10^{-3}T$
933.61-1177 K: $\Delta Hf° = -730.362 - 0.216\times10^{-3}T + 4.054\times10^{-6}T^{2} + 902.900T^{-1}$
$\Delta Gf° = -730.362 + 0.216\times10^{-3}T\ln T - 4.054\times10^{-6}T^{2} + 451.450T^{-1} + 152.382\times10^{-3}T$
1177-1200 K: $\Delta Hf° = -755.825 + 1.821\times10^{-3}T + 3.958\times10^{-6}T^{2} + 801.000T^{-1}$
$\Delta Gf° = -755.825 - 1.821\times10^{-3}T\ln T - 3.958\times10^{-6}T^{2} + 400.500T^{-1} + 188.343\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data based on Kelley (250).

$Na_{0.96}Al_{0.96}Si_{2.04}O_6$(dehydrated analcime)
Sodium Aluminum Disilicate, Dehydrated Analcime

[Formation: $0.96Na(c,l) + 0.96Al(c,l) + 2.04Si(c) + 3O_2(g)$ = Dehydrated Analcime(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	39.100	41.040	41.040	0	-706.500	-666.707	488.703
300	39.240	41.280	41.047	.070	-706.509	-666.461	485.510
371	43.763	50.127	41.935	3.039	-706.659	-656.961	387.000
371	43.763	50.127	41.935	3.039	-707.256	-656.961	387.000
400	45.610	53.490	42.653	4.335	-707.273	-653.029	356.794
500	50.440	64.210	45.920	9.145	-707.080	-639.482	279.514
600	54.320	73.760	49.777	14.390	-706.584	-626.004	228.019
700	57.450	82.380	53.830	19.985	-705.861	-612.631	191.270
800	59.920	90.220	57.901	25.855	-704.977	-599.375	163.740
900	61.780	97.390	61.896	31.945	-703.986	-586.232	142.355
933.61	62.207	99.663	63.215	34.029	-703.638	-581.841	136.202
933.61	62.207	99.663	63.215	34.029	-706.115	-581.841	136.202
1000	63.050	103.970	65.775	38.195	-705.376	-573.009	125.229

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 43.330 + 22.050\times10^{-3}T - 9.604\times10^{5}T^{-2}$
$H°-H°_{298} = 43.330\times10^{-3}T + 11.025\times10^{-6}T^{2} + 9.604\times10^{2}T^{-1} - 17.120$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -709.438 + 1.854\times10^{-3}T + 2.670\times10^{-6}T^{2} + 640.564T^{-1}$
$\Delta Gf° = -709.438 - 1.854\times10^{-3}T\ln T - 2.670\times10^{-6}T^{2} + 320.282T^{-1} + 151.076\times10^{-3}T$
371-933.61 K: $\Delta Hf° = -709.811 - 1.077\times10^{-3}T + 7.230\times10^{-6}T^{2} + 727.828T^{-1}$
$\Delta Gf° = -709.811 + 1.077\times10^{-3}T\ln T - 7.230\times10^{-6}T^{2} + 363.914T^{-1} + 136.115\times10^{-3}T$
933.61-1000 K: $\Delta Hf° = -711.028 - 3.955\times10^{-3}T + 8.888\times10^{-6}T^{2} + 711.124T^{-1}$
$\Delta Gf° = -711.028 + 3.955\times10^{-3}T\ln T - 8.888\times10^{-6}T^{2} + 355.562T^{-1} + 119.293\times10^{-3}T$

Source: Data from Johnson (218).

$NaAlSi_3O_8$(albite)
Sodium Aluminum Trisilicate, Albite
[Formation: $Na(c,l,g) + Al(c,l) + 3Si(c) + 4O_2(g) = NaAlSi_3O_8(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	49.050	49.570	49.570	0	-940.500	-887.124	650.271
300	49.230	49.870	49.570	.091	-940.511	-886.791	646.018
371	54.981	60.994	50.701	3.818	-940.783	-874.047	514.880
371	54.981	60.994	50.701	3.818	-941.405	-874.047	514.880
400	57.330	65.220	51.603	5.447	-941.458	-868.780	474.673
500	62.770	78.640	55.704	11.468	-941.364	-850.611	371.797
600	66.610	90.440	60.527	17.948	-940.992	-832.492	303.231
700	69.420	100.930	65.564	24.756	-940.457	-814.451	254.280
800	71.560	110.350	70.589	31.809	-939.825	-796.495	217.590
900	73.240	118.880	75.489	39.052	-939.148	-778.620	189.072
933.61	73.697	121.574	77.100	41.521	-938.913	-772.629	180.863
933.61	73.697	121.574	77.100	41.521	-941.493	-772.629	180.863
1000	74.600	126.670	80.223	46.447	-940.985	-760.614	166.230
1100*	75.740	133.830	84.771	53.965	-940.189	-742.633	147.546
1177	76.487	138.978	88.147	59.827	-939.546	-728.818	135.328
1177	76.487	138.978	88.147	59.827	-962.831	-728.818	135.328
1200	76.710	140.460	89.136	61.589	-962.589	-724.250	131.902
1300	77.560	146.640	93.330	69.303	-961.504	-704.439	118.426
1400	78.330	152.410	97.340	77.098	-960.392	-684.686	106.883

*Data extrapolated above 1000 K.

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 62.781 + 13.060\times10^{-3}T - 15.667\times10^{5}T^{-2}$
$H° - H°_{298} = 62.781\times10^{-3}T + 6.530\times10^{-6}T^{2} + 15.667\times10^{2}T^{-1} - 24.553$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -946.425 + 8.281\times10^{-3}T - 2.920\times10^{-6}T^{2} + 1107.800T^{-1}$
$\Delta Gf° = -946.425 - 8.281\times10^{-3}T\ln T + 2.920\times10^{-6}T^{2} + 553.900T^{-1} + 238.977\times10^{-3}T$
371-933.61 K: $\Delta Hf° = -946.813 + 5.228\times10^{-3}T + 1.830\times10^{-6}T^{2} + 1198.700T^{-1}$
$\Delta Gf° = -946.813 - 5.228\times10^{-3}T\ln T - 1.830\times10^{-6}T^{2} + 599.350T^{-1} + 223.393\times10^{-3}T$
933.61-1177 K: $\Delta Hf° = -948.081 + 2.230\times10^{-3}T + 3.557\times10^{-6}T^{2} + 1181.300T^{-1}$
$\Delta Gf° = -948.081 - 2.230\times10^{-3}T\ln T - 3.557\times10^{-6}T^{2} + 590.650T^{-1} + 205.869\times10^{-3}T$
1177-1400 K: $\Delta Hf° = -973.544 + 4.267\times10^{-3}T + 3.461\times10^{-6}T^{2} + 1079.400T^{-1}$
$\Delta Gf° = -973.544 - 4.267\times10^{-3}T\ln T - 3.461\times10^{-6}T^{2} + 539.700T^{-1} + 241.830\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Hemingway (204). Low-temperature heat capacities and entropy at 298 K from Openshaw (373). High-temperature data based on Hemingway (203).

$NaAlSi_3O_8$(analbite)
Sodium Aluminum Trisilicate, Analbite
[Formation: $Na(c,l,g) + Al(c,l) + 3Si(c) + 4O_2(g) = NaAlSi_3O_8(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	48.950	54.110	54.110	0	-937.900	-885.878	649.357
300	49.120	54.420	54.137	.085	-937.917	-885.562	645.123
371	54.921	65.517	55.240	3.813	-938.188	-873.131	514.340
371	54.921	65.517	55.240	3.813	-938.810	-873.131	514.340
400	57.290	69.740	56.140	5.440	-938.865	-867.995	474.244
500	62.930	83.170	60.250	11.460	-938.772	-850.284	371.654
600	66.870	95.000	65.053	17.968	-938.372	-832.608	303.273
700	69.720	105.540	70.096	24.811	-937.802	-815.023	254.459
800	71.820	115.010	75.144	31.893	-937.141	-797.539	217.875
900	73.400	123.540	80.041	39.149	-936.451	-780.117	189.436
933.61	73.817	126.239	81.656	41.623	-936.211	-774.282	181.250
933.61	73.817	126.239	81.656	41.623	-938.791	-774.282	181.250
1000	74.640	131.360	84.802	46.558	-938.274	-762.593	166.662
1100	75.640	138.530	89.366	54.080	-937.474	-745.088	148.034
1177	76.310	143.641	92.720	59.935	-936.839	-731.600	135.845
1177	76.310	143.641	92.720	59.935	-960.124	-731.600	135.845
1200	76.510	145.120	93.710	61.692	-959.886	-727.139	132.428
1300	77.250	151.290	97.920	69.381	-958.826	-707.806	118.992
1400	77.960	157.050	101.959	77.127	-957.763	-688.553	107.487

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 62.457 + 13.540\times10^{-3}T - 15.595\times10^{5}T^{-2}$

$H°- H°_{298} = 62.457\times10^{-3}T + 6.770\times10^{-6}T^{2} + 15.595\times10^{2}T^{-1} - 24.454$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -943.726 + 7.957\times10^{-3}T - 2.680\times10^{-6}T^{2} + 1100.600T^{-1}$

$\Delta Gf° = -943.726 - 7.957\times10^{-3}T\ln T + 2.680\times10^{-6}T^{2} + 550.300T^{-1} + 232.369\times10^{-3}T$

371-933.61 K: $\Delta Hf° = -944.114 + 4.904\times10^{-3}T + 2.070\times10^{-6}T^{2} + 1191.500T^{-1}$

$\Delta Gf° = -944.114 - 4.904\times10^{-3}T\ln T - 2.070\times10^{-6}T^{2} + 595.750T^{-1} + 216.785\times10^{-3}T$

933.61-1177 K: $\Delta Hf° = -945.382 + 1.906\times10^{-3}T + 3.797\times10^{-6}T^{2} + 1174.100T^{-1}$

$\Delta Gf° = -945.382 - 1.906\times10^{-3}T\ln T - 3.797\times10^{-6}T^{2} + 587.050T^{-1} + 199.262\times10^{-3}T$

1177-1400 K: $\Delta Hf° = -970.844 + 3.943\times10^{-3}T + 3.701\times10^{-6}T^{2} + 1072.200T^{-1}$

$\Delta Gf° = -970.844 - 3.943\times10^{-3}T\ln T - 3.701\times10^{-6}T^{2} + 536.100T^{-1} + 235.223\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Hemingway (204). Other data from Hemingway (203).

$NaAlSi_3O_8$(vitreous)
Sodium Aluminum Trisilicate

[Formation: $Na(c,l,g) + Al(c,l) + 3Si(c) + 4O_2(g) = NaAlSi_3O_8(vit)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	50.170	61.190	61.190	0	-926.500	-876.588	642.548
300	50.530	61.500	61.200	.090	-926.512	-876.281	638.362
371	56.458	72.890	62.357	3.908	-926.694	-864.371	509.180
371	56.458	72.890	62.357	3.908	-927.316	-864.371	509.180
400	58.880	77.230	63.280	5.580	-927.325	-859.451	469.576
500	64.650	91.030	67.470	11.780	-927.052	-842.493	368.249
600	68.610	103.190	72.440	18.450	-926.490	-825.640	300.735
700	71.470	113.990	77.619	25.460	-925.753	-808.889	252.543
800	73.710	123.690	82.790	32.720	-924.914	-792.256	216.432
900	75.690	132.480	87.813	40.200	-924.000	-775.712	188.366
933.61	76.335	135.267	89.472	42.755	-923.679	-770.180	180.290
933.61	76.335	135.267	89.472	42.755	-926.259	-770.180	180.290
1000	77.610	140.560	92.700	47.860	-925.572	-759.091	165.897
1100	79.640	148.050	97.395	55.720	-924.434	-742.520	147.523
1177	81.388	153.490	100.880	61.922	-923.451	-729.804	135.511
1177	81.388	153.490	100.880	61.922	-946.736	-729.804	135.511
1200	81.910	155.070	101.903	63.800	-946.378	-725.571	132.143
1300	84.490	161.730	106.261	72.110	-944.697	-707.249	118.898
1400	87.450	168.090	110.440	80.710	-942.780	-689.026	107.560

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 61.635 + 17.752\times10^{-3}T - 14.897\times10^{5}T^{-2}$
$H°- H°_{298} = 61.635\times10^{-3}T + 8.876\times10^{-6}T^{2} + 14.897\times10^{2}T^{-1} - 24.162$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -932.034 + 7.135\times10^{-3}T - 0.574\times10^{-6}T^{2} + 1030.800T^{-1}$
$\Delta Gf° = -932.034 - 7.135\times10^{-3}T\ln T + 0.574\times10^{-6}T^{2} + 515.400T^{-1} + 220.647\times10^{-3}T$
371-933.61 K: $\Delta Hf° = -932.422 + 4.082\times10^{-3}T + 4.176\times10^{-6}T^{2} + 1121.700T^{-1}$
$\Delta Gf° = -932.422 - 4.082\times10^{-3}T\ln T - 4.176\times10^{-6}T^{2} + 560.850T^{-1} + 205.063\times10^{-3}T$
933.61-1177 K: $\Delta Hf° = -933.689 + 1.084\times10^{-3}T + 5.903\times10^{-6}T^{2} + 1104.300T^{-1}$
$\Delta Gf° = -933.689 - 1.084\times10^{-3}T\ln T - 5.903\times10^{-6}T^{2} + 552.150T^{-1} + 187.539\times10^{-3}T$
1177-1400 K: $\Delta Hf° = -959.152 + 3.121\times10^{-3}T + 5.807\times10^{-6}T^{2} + 1002.400T^{-1}$
$\Delta Gf° = -959.152 - 3.121\times10^{-3}T\ln T - 5.807\times10^{-6}T^{2} + 501.200T^{-1} + 223.500\times10^{-3}T$

Source: Data from Schumm (438).

$Na_{0.96}Al_{0.96}Si_{2.04}O_6 \cdot H_2O$(analcime)
Sodium Aluminum Disilicate Monohydrate, Analcime
[Formation: $0.96Na(c,l) + 0.96Al(c) + 2.04Si(c) + 3.5O_2(g) + H_2(g) = Analcime(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	50.560	54.200	54.200	0	-784.500	-732.021	536.579
300	50.640	54.510	54.200	.095	-784.504	-731.692	533.031
371	54.616	65.628	55.338	3.818	-784.643	-719.179	423.651
371	54.616	65.628	55.338	3.818	-785.240	-719.179	423.651
400	56.240	69.800	56.238	5.425	-785.252	-714.014	390.114
500	62.720	83.050	60.310	11.370	-784.988	-696.226	304.316
600	68.290	95.000	65.108	17.935	-784.250	-678.535	247.153

Phase change: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 26.394 + 69.834 \times 10^{-3}T + 2.973 \times 10^{5}T^{-2}$

$H°-H°_{298} = 26.394 \times 10^{-3}T + 34.917 \times 10^{-6}T^2 - 2.973 \times 10^{2}T^{-1} - 9.976$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -777.212 - 25.153 \times 10^{-3}T + 25.892 \times 10^{-6}T^2 - 623.236T^{-1}$

$\Delta Gf° = -777.212 + 25.153 \times 10^{-3}T\ln T - 25.892 \times 10^{-6}T^2 - 311.618T^{-1} + 19.482 \times 10^{-3}T$

371-600 K: $\Delta Hf° = -777.584 - 28.084 \times 10^{-3}T + 30.452 \times 10^{-6}T^2 - 535.972T^{-1}$

$\Delta Gf° = -777.584 + 28.084 \times 10^{-3}T\ln T - 30.452 \times 10^{-6}T^2 - 267.986T^{-1} + 4.521 \times 10^{-3}T$

Source: Data from Johnson (218).

$NaBF_4$(c,l)
Sodium Tetrafluoroborate
[Formation: $Na(c,l) + B(\beta) + 2F_2(g) = NaBF_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	28.700	34.730	34.730	0	-440.900	-418.281	306.604
300	28.750	34.910	34.730	.055	-440.890	-418.139	304.610
350	30.210	39.440	35.083	1.525	-440.674	-414.366	258.738
371	31.235	41.230	35.381	2.170	-440.577	-412.790	243.164
371	31.235	41.230	35.381	2.170	-441.199	-412.790	243.164
400	32.650	43.620	35.895	3.090	-441.054	-410.576	224.325
450	36.410	47.660	36.971	4.810	-440.699	-406.780	197.557
500	41.710	51.760	38.250	6.755	-440.145	-403.041	176.167
516	43.740	53.110	38.692	7.440	-439.911	-401.859	170.204
516	35.280	56.270	38.692	9.070	-438.281	-401.859	170.204
550	35.820	58.530	39.839	10.280	-438.040	-399.465	158.731
600	36.610	61.680	41.530	12.090	-437.666	-395.974	144.232
650	37.390	64.650	43.204	13.940	-437.270	-392.521	131.976
679	37.850	66.290	44.153	15.030	-437.029	-390.529	125.698
679	39.520	71.000	44.153	18.230	-433.829	-390.529	125.698
700	39.520	72.200	44.971	19.060	-433.616	-389.189	121.509
750	39.520	74.930	46.883	21.035	-433.119	-386.037	112.490
800	39.520	77.480	48.718	23.010	-432.631	-382.914	104.606
850	39.520	79.880	50.480	24.990	-432.147	-379.819	97.657
900	39.520	82.140	52.179	26.965	-431.677	-376.756	91.488

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
516 K, α - β transition point of $NaBF_4$; ΔH° = 1.630 kcal/mol.
679 K, melting point of $NaBF_4$; ΔH° = 3.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-516 K: $Cp^\circ = -20.499 + 111.682\times10^{-3}T + 14.135\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = -20.499\times10^{-3}T + 55.841\times10^{-6}T^2 - 14.135\times10^{2}T^{-1} + 5.889$
516-679 K: $Cp^\circ = 27.170 + 15.724\times10^{-3}T$
$H^\circ - H^\circ_{298} = 27.170\times10^{-3}T + 7.862\times10^{-6}T^2 - 7.043$
679-900 K: $Cp^\circ = 39.520$
$H^\circ - H^\circ_{298} = 39.520\times10^{-3}T - 8.604$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -425.428 - 46.189\times10^{-3}T + 50.143\times10^{-6}T^2 - 1836.000T^{-1}$
$\Delta Gf^\circ = -425.428 + 46.189\times10^{-3}T\ln T - 50.143\times10^{-6}T^2 - 918.000T^{-1} - 213.918\times10^{-3}T$
371-516 K: $\Delta Hf^\circ = -425.816 - 49.242\times10^{-3}T + 54.893\times10^{-6}T^2 - 1745.100T^{-1}$
$\Delta Gf^\circ = -425.816 + 49.242\times10^{-3}T\ln T - 54.893\times10^{-6}T^2 - 872.550T^{-1} - 229.502\times10^{-3}T$
516-679 K: $\Delta Hf^\circ = -438.748 - 1.573\times10^{-3}T + 6.914\times10^{-6}T^2 - 331.600T^{-1}$
$\Delta Gf^\circ = -438.748 + 1.573\times10^{-3}T\ln T - 6.914\times10^{-6}T^2 - 165.800T^{-1} + 65.894\times10^{-3}T$
679-900 K: $\Delta Hf^\circ = -440.309 + 10.777\times10^{-3}T - 0.948\times10^{-6}T^2 - 331.600T^{-1}$
$\Delta Gf^\circ = -440.309 - 10.777\times10^{-3}T\ln T + 0.948\times10^{-6}T^2 - 165.800T^{-1} + 143.384\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (516). Other data based on Dworkin (133).

$NaBH_4(c)$
Sodium Borohydride
[Formation: $Na(c,l) + B(\beta) + 2H_2(g) = NaBH_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	20.670	24.232	24.232	0	-45.850	-30.379	22.268
300	20.708	24.360	24.233	.038	-45.855	-30.282	22.060
371	22.051	28.903	24.702	1.559	-46.037	-26.578	15.656
371	22.051	28.903	24.702	1.559	-46.659	-26.578	15.656
400	22.600	30.583	25.068	2.206	-46.736	-25.005	13.662
500	24.330	35.814	26.708	4.553	-46.935	-19.545	8.543
600	25.960	40.395	28.615	7.068	-47.016	-14.061	5.122
700	27.550	44.517	30.597	9.744	-46.968	-8.570	2.676
770	28.380	47.184	31.984	11.704	-46.862	-4.732	1.343

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
770 K, melting point of $NaBH_4$; ΔH° unknown.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-770 K: $Cp° = 17.054 + 15.170\text{x}10^{-3}T - 0.806\text{x}10^{5}T^{-2}$
$H° - H°_{298} = 17.054\text{x}10^{-3}T + 7.585\text{x}10^{-6}T^{2} + 0.806\text{x}10^{2}T^{-1} - 6.029$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -44.261 - 4.532\text{x}10^{-3}T + 1.397\text{x}10^{-6}T^{2} - 107.900T^{-1}$
$\Delta Gf° = -44.261 + 4.532\text{x}10^{-3}T\ln T - 1.397\text{x}10^{-6}T^{2} - 53.950T^{-1} + 21.763\text{x}10^{-3}T$
371-770 K: $\Delta Hf° = -44.649 - 7.585\text{x}10^{-3}T + 6.147\text{x}10^{-6}T^{2} - 17.000T^{-1}$
$\Delta Gf° = -44.649 + 7.585\text{x}10^{-3}T\ln T - 6.147\text{x}10^{-6}T^{2} - 8.500T^{-1} + 6.179\text{x}10^{-3}T$

Source: Data from JANAF (127).

$NaBO_2(c)$
Sodium Borate
[Formation: $Na(c,l,g) + B(\beta) + O_2(g) = NaBO_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	15.760	17.570	17.570	0	-233.500	-220.041	161.292
300	15.810	17.670	17.573	.029	-233.501	-219.956	160.236
371	17.379	21.198	17.935	1.211	-233.539	-216.748	127.681
371	17.379	21.198	17.935	1.211	-234.161	-216.748	127.681
400	18.020	22.530	18.220	1.724	-234.177	-215.387	117.680
500	19.770	26.750	19.516	3.617	-234.163	-210.687	92.090
600	21.170	30.480	21.035	5.667	-234.064	-206.000	75.035
700	22.300	33.830	22.627	7.842	-233.891	-201.335	62.859
800	23.240	36.870	24.220	10.120	-233.652	-196.698	53.735
900	24.020	39.660	25.788	12.485	-233.360	-192.100	46.648
1000	24.670	42.220	27.300	14.920	-233.030	-187.528	40.984
1100	25.160	44.600	28.770	17.413	-232.676	-183.007	36.360
1177	25.406	46.308	29.857	19.362	-232.395	-179.528	33.335
1177	25.406	46.308	29.857	19.362	-255.680	-179.528	33.335
1200	25.480	46.800	30.177	19.947	-255.550	-178.043	32.426
1240	25.540	47.640	30.731	20.967	-255.322	-175.468	30.926

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1240 K, melting point of $NaBO_2$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1240 K: $Cp^\circ = 17.780 + 7.160\times10^{-3}T - 3.700\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.780\times10^{-3}T + 3.580\times10^{-6}T^{2} + 3.700\times10^{2}T^{-1} - 6.860$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -234.204 + 1.876\times10^{-3}T - 2.273\times10^{-6}T^{2} + 103.300T^{-1}$
$\Delta Gf^\circ = -234.204 - 1.876\times10^{-3}T\ln T + 2.273\times10^{-6}T^{2} + 51.650T^{-1} + 56.933\times10^{-3}T$
371-1177 K: $\Delta Hf^\circ = -234.592 - 1.177\times10^{-3}T + 2.477\times10^{-6}T^{2} + 194.200T^{-1}$
$\Delta Gf^\circ = -234.592 + 1.177\times10^{-3}T\ln T - 2.477\times10^{-6}T^{2} + 97.100T^{-1} + 41.349\times10^{-3}T$
1177-1240 K: $\Delta Hf^\circ = -260.055 + 0.860\times10^{-3}T + 2.381\times10^{-6}T^{2} + 92.300T^{-1}$
$\Delta Gf^\circ = -260.055 - 0.860\times10^{-3}T\ln T - 2.381\times10^{-6}T^{2} + 46.150T^{-1} + 77.310\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Adami (4). Low-temperature heat capacities and entropy at 298 K from Grenier (183). High-temperature data from Pankratz (385).

$NaB_3O_5(c)$
Sodium Triborate
[Formation: $Na(c,l) + 3B(\beta) + 2.5O_2(g) = NaB_3O_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	29.390	29.000	29.000	0	-550.400	-517.591	379.400
300	29.520	29.180	29.000	.054	-550.406	-517.384	376.909
371	33.908	35.941	29.688	2.320	-550.543	-509.558	300.168
371	33.908	35.941	29.688	2.320	-551.165	-509.558	300.168
400	35.700	38.560	30.238	3.329	-551.201	-506.304	276.628
500	40.420	47.060	32.768	7.146	-551.173	-495.071	216.393
600	43.990	54.760	35.802	11.375	-550.978	-483.874	176.249
700	46.700	61.750	39.014	15.915	-550.643	-472.709	147.585
800	48.870	68.130	42.259	20.697	-550.188	-461.603	126.102
900	50.800	74.000	45.464	25.682	-549.635	-450.561	109.410
1000	52.780	79.460	48.601	30.859	-548.980	-439.593	96.072
1040	53.660	81.540	49.821	32.988	-548.683	-435.216	91.457

*Entropy at 298 K estimated.

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1040 K, melting point of NaB_3O_5; liquid freezes to vitreous form.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1040 K: $Cp^\circ = 32.790 + 21.880\text{x}10^{-3}T - 8.820\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 32.790\text{x}10^{-3}T + 10.940\text{x}10^{-6}T^2 + 8.820\text{x}10^{2}T^{-1} - 13.707$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -549.997 - 3.405\text{x}10^{-3}T + 2.949\text{x}10^{-6}T^2 + 104.500T^{-1}$
$\Delta Gf^\circ = -549.997 + 3.405\text{x}10^{-3}T\ln T - 2.949\text{x}10^{-6}T^2 + 52.250T^{-1} + 89.581\text{x}10^{-3}T$
371-1040 K: $\Delta Hf^\circ = -550.386 - 6.458\text{x}10^{-3}T + 7.699\text{x}10^{-6}T^2 + 195.400T^{-1}$
$\Delta Gf^\circ = -550.386 + 6.458\text{x}10^{-3}T\ln T - 7.699\text{x}10^{-6}T^2 + 97.700T^{-1} + 73.997\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Adami (4). Entropy at 298 K is that estimated by Adami (4). Other data from Pankratz (385).

$Na_2B_4O_7(c)$
Sodium Diborate
[Formation: $2Na(c,l) + 4B(\beta) + 3.5O_2(g) = Na_2B_4O_7(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	44.640	45.296	45.296	0	-786.900	-740.252	542.612
300	44.830	45.572	45.299	.082	-786.908	-739.958	539.052
371	50.979	55.779	46.342	3.501	-787.112	-728.831	429.337
371	50.979	55.779	46.342	3.501	-788.356	-728.831	429.337
400	53.490	59.710	47.170	5.016	-788.415	-724.176	395.666
500	60.170	72.390	50.962	10.714	-788.385	-708.097	309.505
600	65.300	83.840	55.510	16.998	-788.086	-692.079	252.086
700	69.340	94.220	60.309	23.738	-787.553	-676.111	211.089
800	72.730	103.700	65.144	30.845	-786.813	-660.233	180.365
900	75.930	112.450	69.919	38.278	-785.885	-644.462	156.495
1000	79.370	120.630	74.591	46.039	-784.750	-628.811	137.425
1016	79.980	121.890	75.322	47.313	-784.547	-626.314	134.723

Phase changes: 371 K, melting point of Na; $\Delta H^\circ = 0.622$ kcal/mol.
1016 K, melting point of $Na_2B_4O_7$; liquid freezes to vitreous form.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1016 K: $C_p^\circ = 47.740 + 33.640\times10^{-3}T - 11.660\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 47.740\times10^{-3}T + 16.820\times10^{-6}T^{2} + 11.660\times10^{2}T^{-1} - 19.640$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -786.273 - 4.359\times10^{-3}T + 2.976\times10^{-6}T^{2} + 121.800T^{-1}$
$\Delta Gf^\circ = -786.273 + 4.359\times10^{-3}T\ln T - 2.976\times10^{-6}T^{2} + 60.900T^{-1} + 129.722\times10^{-3}T$
371-1016 K: $\Delta Hf^\circ = -787.050 - 10.465\times10^{-3}T + 12.476\times10^{-6}T^{2} + 303.600T^{-1}$
$\Delta Gf^\circ = -787.050 + 10.465\times10^{-3}T\ln T - 12.476\times10^{-6}T^{2} + 151.800T^{-1} + 98.554\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Adami (4). Low-temperature heat capacities and entropy at 298 K from Westrum (527). High-temperature data from Pankratz (385).

$Na_2B_8O_{13}(c)$
Sodium Tetraborate
[Formation: $2Na(c,l) + 8B(\beta) + 6.5O_2(g) = Na_2B_8O_{13}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^\circ_{298})/T$	$H°-H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	73.320	71.000	71.000	0	-1413.600	-1329.102	974.245
300	73.650	71.460	71.007	.136	-1413.613	-1328.569	967.849
371	84.683	88.317	72.714	5.789	-1413.949	-1308.413	770.754
371	84.683	88.317	72.714	5.789	-1415.193	-1308.413	770.754
400	89.190	94.860	74.085	8.310	-1415.277	-1300.063	710.312
500	101.230	116.120	80.404	17.858	-1415.219	-1271.235	555.649
600	110.440	135.430	87.992	28.463	-1414.763	-1242.496	452.573
700	117.460	153.000	96.037	39.874	-1413.965	-1213.828	378.969
800	122.860	169.060	104.184	51.901	-1412.883	-1185.312	323.808
900	127.180	183.780	112.213	64.410	-1411.597	-1156.930	280.937
1000	130.900	197.380	120.062	77.318	-1410.149	-1128.710	246.676
1090	134.080	208.800	126.927	89.242	-1408.726	-1103.495	221.253

*Entropy and heat capacity at 298 K estimated.

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1090 K, melting point of $Na_2B_8O_{13}$; liquid freezes to vitreous form.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1090 K: $Cp° = 82.650 + 54.080\times10^{-3}T - 22.620\times10^{5}T^{-2}$
$H° - H^\circ_{298} = 82.650\times10^{-3}T + 27.040\times10^{-6}T^2 + 22.620\times10^{2}T^{-1} - 34.633$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -1412.060 - 10.031\times10^{-3}T + 8.918\times10^{-6}T^2 + 196.200T^{-1}$
$\Delta Gf° = -1412.060 + 10.031\times10^{-3}T\ln T - 8.918\times10^{-6}T^2 + 98.100T^{-1} + 222.647\times10^{-3}T$
371-1090 K: $\Delta Hf° = -1412.837 - 16.137\times10^{-3}T + 18.419\times10^{-6}T^2 + 378.000T^{-1}$
$\Delta Gf° = -1412.837 + 16.137\times10^{-3}T\ln T - 18.419\times10^{-6}T^2 + 189.000T^{-1} + 191.480\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Adami (4). Entropy and heat capacity at 298 K estimated. High-temperature data from Pankratz (385).

$Na_2C_2(c)$
Disodium Acetylide
[Formation: $2Na(c,l) + 2C(c) = Na_2C_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	21.745	26.587	26.587	0	4.800	5.025	-3.683
300*	21.780	26.720	26.587	.040	4.808	5.027	-3.662
371	23.115	31.490	27.092	1.632	5.063	5.044	-2.971
371	23.115	31.490	27.092	1.632	3.819	5.044	-2.971
400	23.660	33.250	27.475	2.310	3.902	5.137	-2.807
500	25.400	38.720	29.180	4.770	4.246	5.414	-2.366
546	26.170	40.990	30.093	5.950	4.425	5.507	-2.204
546	26.170	42.840	30.093	6.960	5.435	5.507	-2.204
600	27.070	45.350	31.350	8.400	5.680	5.506	-2.006
700	28.720	49.640	33.654	11.190	6.210	5.439	-1.698
800	30.350	53.580	35.905	14.140	6.852	5.286	-1.444
900	31.970	57.250	38.072	17.260	7.618	5.046	-1.225
1000	33.590	60.710	40.170	20.540	8.504	4.708	-1.029
1100	35.210	63.980	42.180	23.980	9.504	4.308	-.856

*Data above 298 K estimated except temperature of fusion.

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
546 K, α - β transition point of Na_2C_2; ΔH° = 1.010 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-546 K: $Cp^\circ = 17.610 + 16.040\times10^{-3}T - 0.578\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.610\times10^{-3}T + 8.020\times10^{-6}T^{2} + 0.578\times10^{2}T^{-1} - 6.157$
546-1100 K: $Cp^\circ = 17.610 + 16.040\times10^{-3}T - 0.578\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.610\times10^{-3}T + 8.020\times10^{-6}T^{2} + 0.578\times10^{2}T^{-1} - 5.152$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = 5.217 + 2.672\times10^{-3}T - 2.828\times10^{-6}T^{2} - 286.800T^{-1}$
$\Delta Gf^\circ = 5.217 - 2.672\times10^{-3}T\ln T + 2.828\times10^{-6}T^{2} - 143.400T^{-1} + 15.349\times10^{-3}T$
371-546 K: $\Delta Hf^\circ = 4.440 - 3.434\times10^{-3}T + 6.672\times10^{-6}T^{2} - 105.000T^{-1}$
$\Delta Gf^\circ = 4.440 + 3.434\times10^{-3}T\ln T - 6.672\times10^{-6}T^{2} - 52.500T^{-1} - 15.818\times10^{-3}T$
546-1100 K: $\Delta Hf^\circ = 5.450 - 3.434\times10^{-3}T + 6.672\times10^{-6}T^{2} - 105.000T^{-1}$
$\Delta Gf^\circ = 5.450 + 3.434\times10^{-3}T\ln T - 6.672\times10^{-6}T^{2} - 52.500T^{-1} - 17.668\times10^{-3}T$

Source: Data from Johnson (221) who estimated all above 298 K except temperature of fusion.

NaCN(c,l,g)
Sodium Cyanide
[Formation: $Na(c,l,g) + C(c) + 0.5N_2(g) = NaCN(c,l,g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	16.415	28.315	28.315	0	-20.910	-18.453	13.526
300	16.390	28.416	28.316	.030	-20.902	-18.438	13.432
371*	16.404	31.906	28.682	1.196	-20.652	-17.884	10.535
371	16.404	31.906	28.682	1.196	-21.274	-17.884	10.535
400	16.410	33.141	28.961	1.672	-21.197	-17.622	9.628
500	16.432	36.805	30.175	3.315	-20.963	-16.755	7.324
600	16.455	39.803	31.538	4.959	-20.774	-15.932	5.803
700	16.478	42.341	32.904	6.606	-20.621	-15.139	4.726
800	16.502	44.543	34.224	8.255	-20.497	-14.363	3.924
835	16.510	45.249	34.657	8.844	-20.449	-14.084	3.686
835	19.000	47.764	34.657	10.944	-18.349	-14.084	3.686
900	19.000	49.188	35.656	12.179	-18.130	-13.761	3.342
1000	19.000	51.190	37.111	14.079	-17.814	-13.293	2.905
1100	19.000	53.001	38.475	15.979	-17.528	-12.846	2.552
1177	19.000	54.286	39.467	17.442	-17.326	-12.531	2.327
1177	19.000	54.286	39.467	17.442	-40.611	-12.531	2.327
1200	19.000	54.654	39.755	17.879	-40.507	-11.986	2.183
1300	19.000	56.175	40.960	19.779	-40.059	-9.625	1.618
1400	19.000	57.583	42.098	21.679	-39.625	-7.301	1.140
1500	19.000	58.894	43.175	23.579	-39.205	-5.008	.730
1600	19.000	60.120	44.196	25.479	-38.793	-2.741	.374
1700	19.000	61.272	45.167	27.379	-38.394	-.502	.065
1800	19.000	62.358	46.092	29.279	-38.002	1.717	-.208
1900	19.000	63.385	46.975	31.179	-37.618	3.914	-.450
1941.2	19.000	63.793	47.328	31.962	-37.461	4.812	-.542
1941.2	14.498	83.093	47.328	69.428	.005	4.812	-.542
2000	14.520	83.527	48.387	70.281	-.040	4.957	-.542

*Data above 346 K estimated except temperature of fusion.

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
835 K, melting point of NaCN; ΔH° = 2.100 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1941.2 K, calculated boiling point of NaCN; ΔH° = 37.466 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-835 K: $Cp^\circ = 15.978 + 0.738\times10^{-3}T + 0.193\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 15.978\times10^{-3}T + 0.369\times10^{-6}T^2 - 0.193\times10^{2}T^{-1} - 4.732$
835-1941.2 K: $Cp^\circ = 19.000$
$H^\circ - H^\circ_{298} = 19.000\times10^{-3}T - 4.921$
1941.2-2000 K: $Cp^\circ = 13.770 + 0.374\times10^{-3}T$
$H^\circ - H^\circ_{298} = 13.770\times10^{-3}T + 0.187\times10^{-6}T^2 + 41.993$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -21.371 + 5.250\times10^{-3}T - 5.349\times10^{-6}T^2 - 187.650T^{-1}$
$\Delta Gf^\circ = -21.371 - 5.250\times10^{-3}T\ln T + 5.349\times10^{-6}T^2 - 93.825T^{-1} + 39.160\times10^{-3}T$
371-835 K: $\Delta Hf^\circ = -21.759 + 2.197\times10^{-3}T - 0.600\times10^{-6}T^2 - 96.750T^{-1}$
$\Delta Gf^\circ = -21.759 - 2.197\times10^{-3}T\ln T + 0.600\times10^{-6}T^2 - 48.375T^{-1} + 23.576\times10^{-3}T$
835-1177 K: $\Delta Hf^\circ = -21.948 + 5.219\times10^{-3}T - 0.969\times10^{-6}T^2 - 77.450T^{-1}$
$\Delta Gf^\circ = -21.948 - 5.219\times10^{-3}T\ln T + 0.969\times10^{-6}T^2 - 38.725T^{-1} + 43.811\times10^{-3}T$
1177-1941.2 K: $\Delta Hf^\circ = -47.411 + 7.256\times10^{-3}T - 1.065\times10^{-6}T^2 - 179.350T^{-1}$
$\Delta Gf^\circ = -47.411 - 7.256\times10^{-3}T\ln T + 1.065\times10^{-6}T^2 - 89.675T^{-1} + 79.772\times10^{-3}T$
1941.2-2000 K: $\Delta Hf^\circ = -0.497 + 2.027\times10^{-3}T - 0.878\times10^{-6}T^2 - 179.350T^{-1}$
$\Delta Gf^\circ = -0.497 - 2.027\times10^{-3}T\ln T + 0.878\times10^{-6}T^2 - 89.675T^{-1} + 16.371\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127) who estimated all above 346 K except temperature of fusion.

NaCN(g)
Sodium Cyanide (ideal gas)
[Formation: Na(c,l,g) + C(c) + $0.5N_2(g)$ = NaCN(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	11.993	58.139	58.139	0	26.000	19.565	-14.341
300	12.003	58.213	58.140	.022	26.000	19.525	-14.224
371	12.298	60.799	58.409	.887	25.949	17.997	-10.602
371	12.298	60.799	58.409	.887	25.327	17.997	-10.602
400	12.419	61.729	58.617	1.245	25.286	17.426	-9.521
500	12.707	64.532	59.528	2.502	25.134	15.478	-6.765
600	12.960	66.872	60.562	3.786	24.963	13.563	-4.940
700	13.194	68.887	61.611	5.093	24.777	11.676	-3.645
800	13.405	70.663	62.633	6.424	24.582	9.820	-2.683
900	13.592	72.253	63.615	7.774	24.376	7.986	-1.939
1000	13.754	73.694	64.553	9.141	24.158	6.175	-1.350
1100	13.893	75.011	65.444	10.524	23.927	4.398	-.874
1177	13.985	75.954	66.101	11.597	23.739	3.031	-.563
1177	13.985	75.954	66.101	11.597	.454	3.031	-.563
1200	14.012	76.225	66.292	11.919	.443	3.079	-.561
1300	14.113	77.351	67.100	13.326	.398	3.303	-.555
1400	14.200	78.400	67.871	14.741	.347	3.527	-.551
1500	14.274	79.382	68.605	16.165	.292	3.756	-.547
1600	14.338	80.306	69.309	17.596	.234	3.989	-.545
1700	14.393	81.177	69.982	19.032	.169	4.223	-.543
1800	14.441	82.001	70.627	20.474	.103	4.464	-.542
1900	14.483	82.783	71.246	21.921	.035	4.709	-.542
2000	14.520	83.527	71.841	23.371	-.039	4.957	-.542

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:

$$C_p^\circ = 12.473 + 1.240\times10^{-3}T - 0.755\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 12.473\times10^{-3}T + 0.620\times10^{-6}T^{2} + 0.755\times10^{2}T^{-1} - 4.027$$

Formation equations (kcal/mol):

298.15-371 K:

$$\Delta Hf^\circ = 26.244 + 1.745\times10^{-3}T - 5.098\times10^{-6}T^{2} - 92.850T^{-1}$$

$$\Delta Gf^\circ = 26.244 - 1.745\times10^{-3}T\ln T + 5.098\times10^{-6}T^{2} - 46.425T^{-1} - 13.456\times10^{-3}T$$

371-1177 K:

$$\Delta Hf^\circ = 25.856 - 1.308\times10^{-3}T - 0.349\times10^{-6}T^{2} - 1.950T^{-1}$$

$$\Delta Gf^\circ = 25.856 + 1.308\times10^{-3}T\ln T + 0.349\times10^{-6}T^{2} - 0.975T^{-1} - 29.040\times10^{-3}T$$

1177-2000 K:

$$\Delta Hf^\circ = 0.393 + 0.729\times10^{-3}T - 0.445\times10^{-6}T^{2} - 103.850T^{-1}$$

$$\Delta Gf^\circ = 0.393 - 0.729\times10^{-3}T\ln T + 0.445\times10^{-6}T^{2} - 51.925T^{-1} + 6.921\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data are those estimated by JANAF (127).

$Na_2CO_3(c,l)$
Sodium Carbonate
[Formation: $2Na(c,l,g) + C(c) + 1.5O_2(g) = Na_2CO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	26.840	32.260	32.260	0	-269.880	-249.840	183.135
300	27.030	32.426	32.260	.050	-269.878	-249.714	181.914
371	29.600	38.428	32.877	2.059	-269.793	-244.951	144.295
371	29.600	38.428	32.877	2.059	-271.037	-244.951	144.295
400	30.650	40.695	33.362	2.933	-270.991	-242.913	132.720
500	34.650	47.977	35.583	6.197	-270.623	-235.936	103.126
600	38.500	54.633	38.183	9.870	-269.902	-229.042	83.428
700	44.830	60.859	41.016	13.890	-268.884	-222.337	69.416
723.15	45.985	62.336	41.675	14.941	-268.535	-220.803	66.730
723.15	34.297	62.564	41.675	15.106	-268.370	-220.803	66.730
800	36.650	66.151	43.855	17.837	-267.983	-215.766	58.944
900	39.730	70.645	46.584	21.655	-267.254	-209.280	50.820
1000	42.830	74.991	49.209	25.782	-266.254	-202.891	44.341
1100	45.900	79.218	51.745	30.220	-264.991	-196.605	39.061
1123.15	46.611	80.181	52.321	31.291	-264.661	-195.168	37.977
1123.15	45.300	86.494	52.321	38.381	-257.571	-195.168	37.977
1177	45.300	88.615	53.934	40.820	-256.862	-192.196	35.687
1177	45.300	88.615	53.934	40.820	-303.432	-192.196	35.687
1200	45.300	89.492	54.607	41.862	-303.040	-190.030	34.609
1300	45.300	93.118	57.432	46.392	-301.337	-180.678	30.374
1400	45.300	96.475	60.102	50.922	-299.656	-171.461	26.766
1500	45.300	99.601	62.633	55.452	-297.993	-162.366	23.656
1600	45.300	102.524	65.035	59.982	-296.346	-153.376	20.950
1700	45.300	105.270	67.322	64.512	-294.715	-144.491	18.575
1800	45.300	107.860	69.503	69.042	-293.098	-135.701	16.476
1900	45.300	110.309	71.587	73.572	-291.495	-127.000	14.608
2000	45.300	112.632	73.581	78.102	-289.906	-118.382	12.936

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
723.15 K, α - β transition point of Na_2CO_3; ΔH° = 0.165 kcal/mol.
1123.15 K, melting point of Na_2CO_3; ΔH° = 7.090 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-723.15 K: $Cp^\circ = 13.880 + 41.090\times10^{-3}T + 0.630\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 13.880\times10^{-3}T + 20.545\times10^{-6}T^2 - 0.630\times10^{2}T^{-1} - 5.753$
723.15-1123.15 K: $Cp^\circ = 10.067 + 32.206\times10^{-3}T + 5.396\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.067\times10^{-3}T + 16.103\times10^{-6}T^2 - 5.396\times10^{2}T^{-1} + 0.151$
1123.15-2000 K: $Cp^\circ = 45.300$
$H^\circ - H^\circ_{298} = 45.300\times10^{-3}T - 12.498$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -267.226 - 8.385\times10^{-3}T + 9.708\times10^{-6}T^2 - 303.100T^{-1}$
$\Delta Gf^\circ = -267.226 + 8.385\times10^{-3}T\ln T - 9.708\times10^{-6}T^2 - 151.550T^{-1} + 15.140\times10^{-3}T$
371-723.15 K: $\Delta Hf^\circ = -268.003 - 14.491\times10^{-3}T + 19.208\times10^{-6}T^2 - 121.300T^{-1}$
$\Delta Gf^\circ = -268.003 + 14.491\times10^{-3}T\ln T - 19.208\times10^{-6}T^2 - 60.650T^{-1} - 16.027\times10^{-3}T$
723.15-1123.15 K: $\Delta Hf^\circ = -262.098 - 18.304\times10^{-3}T + 14.767\times10^{-6}T^2 - 597.900T^{-1}$
$\Delta Gf^\circ = -262.098 + 18.304\times10^{-3}T\ln T - 14.767\times10^{-6}T^2 - 298.950T^{-1} - 52.052\times10^{-3}T$
1123.15-1177 K: $\Delta Hf^\circ = -274.747 + 16.929\times10^{-3}T - 1.337\times10^{-6}T^2 - 58.300T^{-1}$
$\Delta Gf^\circ = -274.747 - 16.929\times10^{-3}T\ln T + 1.337\times10^{-6}T^2 - 29.150T^{-1} + 188.383\times10^{-3}T$
1177-2000 K: $\Delta Hf^\circ = -325.673 + 21.003\times10^{-3}T - 1.528\times10^{-6}T^2 - 262.100T^{-1}$
$\Delta Gf^\circ = -325.673 - 21.003\times10^{-3}T\ln T + 1.528\times10^{-6}T^2 - 131.050T^{-1} + 260.304\times10^{-3}T$

Source: Data from Chang (74).

$NaClO_3$(c,l)
Sodium Chlorate
[Formation: $Na(c,l) + 0.5Cl_2(g) + 1.5O_2(g) = NaClO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.930	29.500	29.500	0	-87.422	-62.690	45.953
300	24.010	29.650	29.517	.040	-87.421	-62.541	45.560
350	26.060	33.500	29.786	1.300	-87.244	-58.397	36.465
371	26.896	35.043	30.040	1.856	-87.154	-56.669	33.382
371	26.896	35.043	30.040	1.856	-87.776	-56.669	33.382
400	28.050	37.110	30.485	2.650	-87.635	-54.246	29.638
450	30.010	40.530	31.419	4.100	-87.314	-50.092	24.328
500	31.950	43.790	32.490	5.650	-86.899	-45.975	20.096
528	33.030	45.560	33.137	6.560	-86.627	-43.692	18.085
528	30.200	55.790	33.137	11.960	-81.227	-43.692	18.085
550	30.200	57.020	34.075	12.620	-81.070	-42.134	16.742
600	30.200	59.650	36.100	14.130	-80.707	-38.612	14.064

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
528 K, melting point of $NaClO_3$; ΔH° = 5.400 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-528 K: $Cp° = 13.153 + 37.972\times10^{-3}T - 0.469\times10^{5}T^{-2}$
$H°- H°_{298} = 13.153\times10^{-3}T + 18.986\times10^{-6}T^{2} + 0.469\times10^{2}T^{-1} - 5.767$
528-600 K: $Cp° = 30.200$
$H°- H°_{298} = 30.200\times10^{-3}T - 3.986$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -86.634 - 6.057\times10^{-3}T + 13.530\times10^{-6}T^{2} - 55.050T^{-1}$
$\Delta Gf° = -86.634 + 6.057\times10^{-3}T\ln T - 13.530\times10^{-6}T^{2} - 27.525T^{-1} + 50.144\times10^{-3}T$
371-528 K: $\Delta Hf° = -87.022 - 9.110\times10^{-3}T + 18.280\times10^{-6}T^{2} + 35.850T^{-1}$
$\Delta Gf° = -87.022 + 9.110\times10^{-3}T\ln T - 18.280\times10^{-6}T^{2} + 17.925T^{-1} + 34.561\times10^{-3}T$
528-600 K: $\Delta Hf° = -85.241 + 7.938\times10^{-3}T - 0.706\times10^{-6}T^{2} - 11.050T^{-1}$
$\Delta Gf° = -85.241 - 7.938\times10^{-3}T\ln T + 0.706\times10^{-6}T^{2} - 5.525T^{-1} + 128.116\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (516). Low-temperature heat capacities from Fransson (156). High-temperature data based on Goodwin (177), Kelley (243), and Campbell (66).

$NaClO_4(c)$
Sodium Perchlorate
[Formation: $Na(c,l) + 0.5Cl_2(g) + 2O_2(g) = NaClO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	26.290	34.390	34.390	0	-91.610	-61.031	44.736
300	26.460	34.570	34.393	.053	-91.603	-60.841	44.322
350	29.160	38.850	34.739	1.439	-91.476	-55.728	34.798
371	30.403	40.585	35.021	2.064	-91.392	-53.585	31.566
371	30.403	40.585	35.021	2.064	-92.014	-53.585	31.566
400	32.120	42.930	35.513	2.967	-91.868	-50.588	27.640
450	36.280	46.930	36.561	4.666	-91.478	-45.449	22.073
500	44.020	51.080	37.800	6.640	-90.824	-40.365	17.643
550	57.720	55.970	39.217	9.214	-89.578	-35.371	14.055
579.2	69.790	59.050	40.164	10.940	-88.632	-32.532	12.275
579.2	40.150	59.590	40.164	11.250	-88.322	-32.532	12.275
600	38.410	60.990	40.870	12.072	-88.058	-30.538	11.123
650	37.280	64.010	42.521	13.968	-87.508	-25.758	8.660

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
579.2 K, α - β transition point of $NaClO_4$; ΔH° = 0.310 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-579.2 K: $Cp° = -64.937 + 199.518\times10^{-3}T + 28.216\times10^{5}T^{-2}$
$H°-H°_{298} = -64.937\times10^{-3}T + 99.759\times10^{-6}T^{2} - 28.216\times10^{2}T^{-1} + 19.957$
579.2-650 K: $Cp° = 66.155 - 45.176\times10^{-3}T$
$H°-H°_{298} = 66.155\times10^{-3}T - 22.588\times10^{-6}T^{2} - 19.489$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -63.923 - 87.761\times10^{-3}T + 94.051\times10^{-6}T^{2} - 2946.150T^{-1}$
$\Delta Gf° = -63.923 + 87.761\times10^{-3}T\ln T - 94.051\times10^{-6}T^{2} - 1473.075T^{-1} - 445.717\times10^{-3}T$
371-579.2 K: $\Delta Hf° = -64.311 - 90.814\times10^{-3}T + 98.801\times10^{-6}T^{2} - 2855.250T^{-1}$
$\Delta Gf° = -64.311 + 90.814\times10^{-3}T\ln T - 98.801\times10^{-6}T^{2} - 1427.625T^{-1} - 461.301\times10^{-3}T$
579.2-650 K: $\Delta Hf° = -103.757 + 40.278\times10^{-3}T - 23.546\times10^{-6}T^{2} - 33.650T^{-1}$
$\Delta Gf° = -103.757 - 40.278\times10^{-3}T\ln T + 23.546\times10^{-6}T^{2} - 16.825T^{-1} + 365.696\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Zalukaev (539). High-temperature data based on Schmidt (446).

$Na_2CrO_4(c,l)$
Sodium Chromate
[Formation: $2Na(c,l,g) + Cr(c) + 2O_2(g) = Na_2CrO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	33.968	42.212	42.212	0	-320.800	-295.146	216.345
300	34.052	42.423	42.213	.063	-320.797	-294.986	214.895
311.5	34.462	43.712	42.245	.457	-320.788	-293.997	206.267
371	36.585	49.922	42.986	2.573	-320.696	-288.887	170.176
371	36.585	49.922	42.986	2.573	-321.940	-288.887	170.176
400	37.620	52.714	43.591	3.649	-321.900	-286.305	156.428
500	40.950	61.467	46.311	7.578	-321.537	-277.438	121.267
600	44.410	69.235	49.495	11.844	-320.881	-268.674	97.863
700	48.140	76.357	52.831	16.468	-319.912	-260.047	81.189
700	45.540	79.589	52.831	18.731	-317.649	-260.047	81.189
800	45.840	85.678	56.564	23.291	-316.787	-251.878	68.809
900	47.200	91.145	60.107	27.934	-315.882	-243.816	59.206
1000	49.630	96.235	63.468	32.767	-314.835	-235.866	51.548
1065	51.780	99.425	65.565	36.061	-314.040	-230.758	47.353
1065	50.440	104.881	65.565	41.871	-308.230	-230.758	47.354
1100	50.440	106.512	66.842	43.637	-307.821	-228.218	45.342
1177	50.440	109.925	69.550	47.521	-306.952	-222.664	41.345
1177	50.440	109.925	69.550	47.521	-353.522	-222.664	41.345
1200	50.440	110.901	70.334	48.681	-353.179	-220.115	40.088
1300	50.440	114.938	73.611	53.725	-351.710	-209.090	35.151
1400	50.440	118.676	76.699	58.768	-350.298	-198.180	30.937

Phase changes: 311.5 K, second-order transition point of Cr; $\Delta H^\circ = 0$ kcal/mol.
371 K, melting point of Na; $\Delta H^\circ = 0.622$ kcal/mol.
700 K, $\alpha - \beta$ transition point of Na_2CrO_4; ΔH° 2.263 kcal/mol.
1065 K, melting point of Na_2CrO_4; $\Delta H^\circ = 5.810$ kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; $\Delta H^\circ = 23.285$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $C_p^\circ = 24.403 + 33.604\times10^{-3}T - 0.403\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 24.403\times10^{-3}T + 16.802\times10^{-6}T^2 + 0.403\times10^{2}T^{-1} - 8.905$
700-1065 K: $C_p^\circ = 1.030 + 40.700\times10^{-3}T + 78.510\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 1.030\times10^{-3}T + 20.350\times10^{-6}T^2 - 78.510\times10^{2}T^{-1} + 19.254$
1065-1400 K: $C_p^\circ = 50.440$
$H^\circ - H^\circ_{298} = 50.440\times10^{-3}T - 11.848$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -321.403 + 4.849\times10^{-3}T - 7.587\times10^{-6}T^2 - 50.100T^{-1}$
$\Delta Gf^\circ = -321.403 - 4.849\times10^{-3}T\ln T + 7.587\times10^{-6}T^2 - 25.050T^{-1} + 113.715\times10^{-3}T$
311.5-371 K: $\Delta Hf^\circ = -320.406 - 2.318\times10^{-3}T + 4.689\times10^{-6}T^2 - 36.500T^{-1}$
$\Delta Gf^\circ = -320.406 + 2.318\times10^{-3}T\ln T - 4.689\times10^{-6}T^2 - 18.250T^{-1} + 73.117\times10^{-3}T$
371-700 K: $\Delta Hf^\circ = -321.182 - 8.424\times10^{-3}T + 14.189\times10^{-6}T^2 + 145.300T^{-1}$
$\Delta Gf^\circ = -321.182 + 8.424\times10^{-3}T\ln T - 14.189\times10^{-6}T^2 + 72.650T^{-1} + 41.949\times10^{-3}T$
700-1065 K: $\Delta Hf^\circ = -293.023 - 31.797\times10^{-3}T + 17.737\times10^{-6}T^2 - 7746.000T^{-1}$
$\Delta Gf^\circ = -293.023 + 31.797\times10^{-3}T\ln T - 17.737\times10^{-6}T^2 - 3873.000T^{-1} - 140.860\times10^{-3}T$
1065-1177 K: $\Delta Hf^\circ = -324.125 + 17.613\times10^{-3}T - 2.613\times10^{-6}T^2 + 105.000T^{-1}$
$\Delta Gf^\circ = -324.125 - 17.613\times10^{-3}T\ln T + 2.613\times10^{-6}T^2 + 52.500T^{-1} + 207.634\times10^{-3}T$
1177-1400 K: $\Delta Hf^\circ = -375.051 + 21.687\times10^{-3}T - 2.805\times10^{-6}T^2 - 98.800T^{-1}$
$\Delta Gf^\circ = -375.051 - 21.687\times10^{-3}T\ln T + 2.805\times10^{-6}T^2 - 49.400T^{-1} + 279.555\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from Ferrante (147).

$NaFeO_2(c,l)$
Sodium Ferrite
[Formation: $Na(c,l,g) + Fe(c,l) + O_2(g) = NaFeO_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$ΔHf°$	$ΔGf°$	
298.15	20.200	21.140	21.140	0	-166.830	-152.911	112.086
300	20.258	21.265	21.142	.037	-166.829	-152.825	111.331
371	22.020	25.771	21.604	1.546	-166.764	-149.517	88.077
371	22.020	25.771	21.604	1.546	-167.386	-149.517	88.077
400	22.739	27.455	21.968	2.195	-167.351	-148.121	80.929
500	24.322	32.712	23.604	4.554	-167.146	-143.334	62.651
600	25.505	37.253	25.510	7.046	-166.867	-138.597	50.483
700	26.856	41.280	27.479	9.661	-166.531	-133.911	41.808
800	28.947	44.992	29.440	12.442	-166.108	-129.281	35.317
880	31.542	47.864	30.983	14.855	-165.656	-125.617	31.197
880	27.088	47.864	30.983	14.855	-165.656	-125.617	31.197
900	27.183	48.474	31.365	15.398	-165.618	-124.708	30.283
1000	27.657	51.363	33.223	18.140	-165.529	-120.170	26.263
1043	27.861	52.532	33.995	19.334	-165.627	-118.218	24.771
1100	28.131	54.021	34.995	20.929	-165.607	-115.627	22.973
1177	28.496	55.936	36.302	23.109	-165.423	-112.131	20.821
1177	28.496	55.936	36.302	23.109	-188.708	-112.131	20.821
1185	28.534	56.130	36.436	23.337	-188.668	-111.611	20.584
1185	28.534	56.130	36.436	23.337	-188.883	-111.611	20.584
1200	28.605	56.489	36.684	23.766	-188.780	-110.636	20.149
1270	28.937	58.121	37.822	25.780	-188.283	-106.090	18.256
1270	28.800	58.530	37.822	26.300	-187.763	-106.090	18.256
1300	28.800	59.202	38.307	27.164	-187.554	-104.162	17.511
1400	28.800	61.336	39.876	30.044	-186.876	-97.773	15.263
1500	28.800	63.323	41.374	32.924	-186.224	-91.433	13.322
1600	28.800	65.182	42.805	35.804	-185.599	-85.133	11.629
1620	28.800	65.540	43.083	36.380	-185.477	-83.879	11.316
1620	37.300	72.799	43.083	48.140	-173.717	-83.879	11.316
1667	37.300	73.866	43.936	49.893	-173.035	-81.283	10.656
1667	37.300	73.866	43.936	49.893	-173.235	-81.283	10.656
1700	37.300	74.597	44.524	51.124	-172.785	-79.467	10.216
1800	37.300	76.729	46.255	54.854	-171.440	-74.015	8.987
1811	37.300	76.956	46.440	55.264	-171.297	-73.423	8.861
1811	37.300	76.956	46.440	55.264	-174.597	-73.423	8.861
1900	37.300	78.746	47.912	58.584	-173.495	-68.478	7.877
2000	37.300	80.659	49.502	62.314	-172.261	-62.983	6.882

Phase changes:
371 K, melting point of Na; $ΔH° = 0.622$ kcal/mol.
880 K, α - β transition point of $NaFeO_2$; $ΔH° = 0$ kcal/mol.
1043 K, Curie temperature of Fe; $ΔH° = 0$ kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; $ΔH° = 23.285$ kcal/mol.
1185 K, α - γ transition point of Fe; $ΔH° = 0.215$ kcal/mol.
1270 K, β - γ transition point of $NaFeO_2$; $ΔH° = 0.520$ kcal/mol.
1620 K, melting point of $NaFeO_2$; $ΔH° = 11.760$ kcal/mol.
1667 K, γ - δ transition point of Fe; $ΔH° = 0.200$ kcal/mol.
1811 K, melting point of Fe; $ΔH° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-880 K: $Cp° = 18.691 + 12.966\text{x}10^{-3}T - 2.097\text{x}10^{5}T^{-2}$
$H° - H°_{298} = 18.691\text{x}10^{-3}T + 6.483\text{x}10^{-6}T^{2} + 2.097\text{x}10^{2}T^{-1} - 6.852$
880-1270 K: $Cp° = 23.143 + 4.592\text{x}10^{-3}T - 0.741\text{x}10^{5}T^{-2}$
$H° - H°_{298} = 23.143\text{x}10^{-3}T + 2.296\text{x}10^{-6}T^{2} + 0.741\text{x}10^{2}T^{-1} - 7.373$
1270-1620 K: $Cp° = 28.800$
$H° - H°_{298} = 28.800\text{x}10^{-3}T - 10.276$
1620-2000 K: $Cp° = 37.300$
$H° - H°_{298} = 37.300\text{x}10^{-3}T - 12.286$

Formation equations (kcal/mol):

298.15-371 K: $ΔHf° = -170.031 + 7.731\text{x}10^{-3}T - 4.749\text{x}10^{-6}T^{2} + 393.000T^{-1}$
$ΔGf° = -170.031 - 7.731\text{x}10^{-3}T\ln T + 4.749\text{x}10^{-6}T^{2} + 196.500T^{-1} + 97.841\text{x}10^{-3}T$
371-880 K: $ΔHf° = -170.419 + 4.678\text{x}10^{-3}T + 0.001\text{x}10^{-6}T^{2} + 483.900T^{-1}$
$ΔGf° = -170.419 - 4.678\text{x}10^{-3}T\ln T - 0.001\text{x}10^{-6}T^{2} + 241.950T^{-1} + 82.257\text{x}10^{-3}T$
880-1043 K: $ΔHf° = -170.940 + 9.130\text{x}10^{-3}T - 4.186\text{x}10^{-6}T^{2} + 348.300T^{-1}$
$ΔGf° = -170.940 - 9.130\text{x}10^{-3}T\ln T + 4.186\text{x}10^{-6}T^{2} + 174.150T^{-1} + 109.436\text{x}10^{-3}T$
1043-1177 K: $ΔHf° = -147.380 - 34.851\text{x}10^{-3}T + 16.525\text{x}10^{-6}T^{2} + 119.800T^{-1}$
$ΔGf° = -147.380 + 34.851\text{x}10^{-3}T\ln T - 16.525\text{x}10^{-6}T^{2} + 59.900T^{-1} - 197.108\text{x}10^{-3}T$
+1177-1185 K: $ΔHf° = -172.843 - 32.814\text{x}10^{-3}T + 16.429\text{x}10^{-6}T^{2} + 17.900T^{-1}$
$ΔGf° = -172.843 + 32.814\text{x}10^{-3}T\ln T - 16.429\text{x}10^{-6}T^{2} + 8.950T^{-1} - 161.147\text{x}10^{-3}T$
1185-1270 K: $ΔHf° = -196.456 + 5.441\text{x}10^{-3}T + 0.738\text{x}10^{-6}T^{2} + 136.900T^{-1}$
$ΔGf° = -196.456 - 5.441\text{x}10^{-3}T\ln T - 0.738\text{x}10^{-6}T^{2} + 68.450T^{-1} + 110.893\text{x}10^{-3}T$
1270-1620 K: $ΔHf° = -199.359 + 11.098\text{x}10^{-3}T - 1.558\text{x}10^{-6}T^{2} + 62.800T^{-1}$
$ΔGf° = -199.359 - 11.098\text{x}10^{-3}T\ln T + 1.558\text{x}10^{-6}T^{2} + 31.400T^{-1} + 150.715\text{x}10^{-3}T$
1620-1667 K: $ΔHf° = -201.369 + 19.598\text{x}10^{-3}T - 1.558\text{x}10^{-6}T^{2} + 62.800T^{-1}$
$ΔGf° = -201.369 - 19.598\text{x}10^{-3}T\ln T + 1.558\text{x}10^{-6}T^{2} + 31.400T^{-1} + 214.773\text{x}10^{-3}T$
1667-1811 K: $ΔHf° = -284.264 + 68.095\text{x}10^{-3}T - 11.189\text{x}10^{-6}T^{2} + 47762.000T^{-1}$
$ΔGf° = -284.264 - 68.095\text{x}10^{-3}T\ln T + 11.189\text{x}10^{-6}T^{2} + 23881.000T^{-1} + 599.651\text{x}10^{-3}T$
1811-2000 K: $ΔHf° = -198.414 + 14.103\text{x}10^{-3}T - 0.507\text{x}10^{-6}T^{2} - 56.200T^{-1}$
$ΔGf° = -198.414 - 14.103\text{x}10^{-3}T\ln T + 0.507\text{x}10^{-6}T^{2} - 28.100T^{-1} + 173.853\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Koehler (276). Low-temperature heat capacities and entropy at 298 K from King (260) High-temperature data based on Christensen (93).

$Na_8Fe_2O_7$(c)
Tetrasodium Ferrite

[Formation: 8Na(c,l,g) + 2Fe(c) + 3.5O_2(g) = $Na_8Fe_2O_7$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	90.575	104.676	104.676	0	-656.200	-603.050	442.042
300	90.744	105.237	104.677	.168	-656.195	-602.715	439.072
371	95.248	124.980	106.721	6.774	-656.248	-590.059	347.589
371	95.248	124.980	106.721	6.774	-661.224	-590.059	347.589
400	97.088	132.218	108.311	9.563	-661.290	-584.492	319.348
500	101.593	154.401	115.377	19.512	-661.191	-565.293	247.086
600	104.643	173.209	123.487	29.833	-660.755	-546.148	198.932
700	107.064	189.525	131.782	40.420	-660.129	-527.103	164.567
800	109.608	203.983	139.921	51.250	-659.382	-508.149	138.818
900	112.762	217.068	147.777	62.362	-658.563	-489.290	118.814
1000	116.566	229.141	155.316	73.825	-657.786	-470.526	102.832
1043	118.222	234.083	158.462	78.873	-657.649	-462.478	96.906
1100	120.416	240.435	162.546	85.678	-657.102	-451.833	89.770
1177	122.315	248.663	167.913	95.043	-655.948	-437.471	81.230
1177	122.315	248.663	167.913	95.043	-842.228	-437.471	81.230
1185	122.512	249.493	168.461	96.023	-841.964	-434.722	80.175
1185	122.512	249.493	168.461	96.023	-842.394	-434.722	80.175
1200	122.882	251.036	169.484	97.863	-841.855	-429.583	78.237

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 90.739 + 26.132\times10^{-3}T - 7.071\times10^{5}T^{-2}$
$H° - H°_{298} = 90.739\times10^{-3}T + 13.066\times10^{-6}T^{2} + 7.071\times10^{2}T^{-1} - 30.587$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -666.404 + 34.268\times10^{-3}T - 38.101\times10^{-6}T^{2} + 1005.900T^{-1}$
$\Delta Gf° = -666.404 - 34.268\times10^{-3}T\ln T + 38.101\times10^{-6}T^{2} + 502.950T^{-1} + 390.717\times10^{-3}T$
371-1043 K: $\Delta Hf° = -669.509 + 9.844\times10^{-3}T - 0.100\times10^{-6}T^{2} + 1733.100T^{-1}$
$\Delta Gf° = -669.509 - 9.844\times10^{-3}T\ln T + 0.100\times10^{-6}T^{2} + 866.550T^{-1} + 266.046\times10^{-3}T$
1043-1177 K: $\Delta Hf° = -622.387 - 78.118\times10^{-3}T + 41.321\times10^{-6}T^{2} + 1276.100T^{-1}$
$\Delta Gf° = -622.387 + 78.118\times10^{-3}T\ln T - 41.321\times10^{-6}T^{2} + 638.050T^{-1} - 347.043\times10^{-3}T$
1177-1185 K: $\Delta Hf° = -826.091 - 61.822\times10^{-3}T + 40.554\times10^{-6}T^{2} + 460.900T^{-1}$
$\Delta Gf° = -826.091 + 61.822\times10^{-3}T\ln T - 40.554\times10^{-6}T^{2} + 230.450T^{-1} - 59.358\times10^{-3}T$
1185-1200 K: $\Delta Hf° = -873.319 + 14.688\times10^{-3}T + 9.172\times10^{-6}T^{2} + 698.900T^{-1}$
$\Delta Gf° = -873.319 - 14.688\times10^{-3}T\ln T - 9.172\times10^{-6}T^{2} + 349.450T^{-1} + 484.723\times10^{-3}T$

Source: Data from Stuve (484).

$NaFe(SiO_3)_2$(acmite)
Sodium Iron Silicate, Acmite

[Formation: $Na(c,l,g) + Fe(c) + 2Si(c) + 3O_2(g) = NaFe(SiO_3)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	40.607	40.622	40.622	0	-615.870	-575.855	422.108
300	40.771	40.874	40.624	.075	-615.875	-575.606	419.323
371	45.115	50.062	41.563	3.153	-615.956	-566.067	333.456
371	45.115	50.062	41.563	3.153	-616.578	-566.067	333.456
400	46.889	53.524	42.306	4.487	-616.577	-562.119	307.123
500	50.959	64.449	45.669	9.390	-616.382	-548.518	239.754
600	53.985	74.020	49.613	14.644	-615.995	-534.981	194.864
700	56.321	82.524	53.717	20.165	-615.491	-521.517	162.823
800	58.153	90.169	57.804	25.892	-614.928	-508.130	138.813
900	59.606	97.106	61.792	31.783	-614.371	-494.813	120.156
1000	60.778	103.449	65.645	37.804	-613.913	-481.540	105.239
1043	61.198	106.017	67.257	40.426	-613.846	-475.850	99.708
1100	61.754	109.289	69.351	43.932	-613.604	-468.329	93.047
1177	62.414	113.489	72.102	48.713	-613.114	-458.172	85.074
1177	62.414	113.489	72.102	48.713	-636.399	-458.172	85.074
1185	62.482	113.912	72.382	49.213	-636.327	-456.961	84.276
1185	62.482	113.912	72.382	49.213	-636.542	-456.961	84.276
1200	62.611	114.699	72.907	50.151	-636.379	-454.692	82.810
1263	63.123	117.916	75.073	54.111	-635.677	-445.170	77.031

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1263 K: $Cp^\circ = 49.038 + 12.722\times10^{-3}T - 10.866\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 49.038\times10^{-3}T + 6.361\times10^{-6}T^{2} + 10.866\times10^{2}T^{-1} - 18.831$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -622.236 + 12.260\times10^{-3}T - 6.579\times10^{-6}T^{2} + 982.500T^{-1}$
$\Delta Gf^\circ = -622.236 - 12.260\times10^{-3}T\ln T + 6.579\times10^{-6}T^{2} + 491.250T^{-1} + 217.927\times10^{-3}T$
371-1043 K: $\Delta Hf^\circ = -622.624 + 9.207\times10^{-3}T - 1.829\times10^{-6}T^{2} + 1073.400T^{-1}$
$\Delta Gf^\circ = -622.624 - 9.207\times10^{-3}T\ln T + 1.829\times10^{-6}T^{2} + 536.700T^{-1} + 202.343\times10^{-3}T$
1043-1177 K: $\Delta Hf^\circ = -599.063 - 34.774\times10^{-3}T + 18.882\times10^{-6}T^{2} + 844.900T^{-1}$
$\Delta Gf^\circ = -599.063 + 34.774\times10^{-3}T\ln T - 18.882\times10^{-6}T^{2} + 422.450T^{-1} - 104.202\times10^{-3}T$
1177-1185 K: $\Delta Hf^\circ = -624.526 - 32.737\times10^{-3}T + 18.786\times10^{-6}T^{2} + 743.000T^{-1}$
$\Delta Gf^\circ = -624.526 + 32.737\times10^{-3}T\ln T - 18.786\times10^{-6}T^{2} + 371.500T^{-1} - 68.241\times10^{-3}T$
1185-1263 K: $\Delta Hf^\circ = -648.140 + 5.518\times10^{-3}T + 3.095\times10^{-6}T^{2} + 862.000T^{-1}$
$\Delta Gf^\circ = -648.140 - 5.518\times10^{-3}T\ln T - 3.095\times10^{-6}T^{2} + 431.000T^{-1} + 203.800\times10^{-3}T$

Source: Data from Bennington (31).

$Na_{0.869}Fe_{0.8962}Mn_{0.03}Ca_{0.1121}Al_{0.141}Si_{1.9738}O_6$(aegirine)

Aegirine

[Formation: 0.869Na(c,l,g) + 0.8962Fe(c) + 0.03Mn(c) + 0.1121Ca(c,l) + 0.141Al(c,l) + 1.9738Si(c) + $3O_2$(g) = Aegirine(c)]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	40.499	38.032	38.032	0	-641.120	-600.365	440.073
300	40.661	38.283	38.033	.075	-641.125	-600.111	437.175
371	44.958	47.448	38.972	3.145	-641.215	-590.395	347.787
371	44.958	47.448	38.972	3.145	-641.756	-590.395	347.787
400	46.713	50.898	39.713	4.474	-641.759	-586.380	320.379
500	50.111	61.719	43.059	9.330	-641.610	-572.544	250.256
600	52.348	71.064	46.966	14.459	-641.352	-558.756	203.524
700	54.136	79.271	51.007	19.785	-641.055	-545.015	170.159
720	54.438	80.800	51.813	20.871	-640.993	-542.272	164.600
720	54.438	80.800	51.813	20.871	-641.018	-542.272	164.600
800	55.647	86.602	55.006	25.277	-640.764	-531.313	145.146
900	56.754	93.225	58.891	30.901	-640.491	-517.646	125.700
933.61	56.927	95.309	60.164	32.811	-640.430	-513.059	120.101
933.61	56.927	95.309	60.164	32.811	-640.794	-513.059	120.101
980	57.165	98.081	61.894	35.464	-640.727	-506.700	112.998
980	57.165	98.081	61.894	35.464	-640.743	-506.700	112.998
1000	57.268	99.237	62.629	36.608	-640.743	-503.965	110.140
1043	57.230	101.647	64.188	39.070	-640.831	-498.082	104.367
1100	57.179	104.695	66.210	42.334	-640.840	-490.295	97.411
1112	57.145	105.315	66.628	43.020	-640.832	-488.654	96.038
1112	57.145	105.315	66.628	43.020	-641.061	-488.654	96.038
1177	56.960	108.555	68.855	46.727	-640.969	-479.745	89.080
1177	56.960	108.555	68.855	46.727	-661.204	-479.745	89.080
1185	56.938	108.941	69.125	47.182	-661.177	-478.512	88.251
1185	56.938	108.941	69.125	47.182	-661.370	-478.512	88.251
1200	56.895	109.657	69.627	48.036	-661.298	-476.200	86.727

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
720 K, α − γ transition point of Ca; ΔH° = 0.220 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
980 K, α − β transition point of Mn; ΔH° = 0.532 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1185 K, α − γ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 51.856 + 6.266x10^{-3}T - 11.756x10^{5}T^{-2}$
$H°-H°_{298} = 51.856x10^{-3}T + 3.133x10^{-6}T^{2} + 11.756x10^{2}T^{-1} - 19.682$

Formation equations (kcal/mol):

298.15-371 K: $ΔHf° = -648.174 + 14.475x10^{-3}T - 9.140x10^{-6}T^{2} + 1058.652T^{-1}$
$ΔGf° = -648.174 - 14.475x10^{-3}TlnT + 9.140x10^{-6}T^{2} + 529.326T^{-1} + 234.149x10^{-3}T$
371-720 K: $ΔHf° = -648.511 + 11.822x10^{-3}T - 5.012x10^{-6}T^{2} + 1137.644T^{-1}$
$ΔGf° = -648.511 - 11.822x10^{-3}TlnT + 5.012x10^{-6}T^{2} + 568.822T^{-1} + 220.606x10^{-3}T$
720-933.61 K: $ΔHf° = -648.706 + 12.264x10^{-3}T - 5.278x10^{-6}T^{2} + 1130.806T^{-1}$
$ΔGf° = -648.706 - 12.264x10^{-3}TlnT + 5.278x10^{-6}T^{2} + 565.403T^{-1} + 223.597x10^{-3}T$
933.61-980 K: $ΔHf° = -648.885 + 11.841x10^{-3}T - 5.035x10^{-6}T^{2} + 1128.352T^{-1}$
$ΔGf° = -648.885 - 11.841x10^{-3}TlnT + 5.035x10^{-6}T^{2} + 564.176T^{-1} + 221.126x10^{-3}T$
980-1043 K: $ΔHf° = -648.873 + 11.776x10^{-3}T - 5.001x10^{-6}T^{2} + 1130.956T^{-1}$
$ΔGf° = -648.873 - 11.776x10^{-3}TlnT + 5.001x10^{-6}T^{2} + 565.478T^{-1} + 220.695x10^{-3}T$
1043-1112 K: $ΔHf° = -627.757 - 27.640x10^{-3}T + 13.561x10^{-6}T^{2} + 926.175T^{-1}$
$ΔGf° = -627.757 + 27.640x10^{-3}TlnT - 13.561x10^{-6}T^{2} + 463.087T^{-1} - 54.030x10^{-3}T$
1112-1177 K: $ΔHf° = -627.785 - 28.437x10^{-3}T + 14.115x10^{-6}T^{2} + 926.175T^{-1}$
$ΔGf° = -627.785 + 28.437x10^{-3}TlnT - 14.115x10^{-6}T^{2} + 463.087T^{-1} - 58.977x10^{-3}T$
1177-1185 K: $ΔHf° = -649.913 - 26.667x10^{-3}T + 14.031x10^{-6}T^{2} + 837.624T^{-1}$
$ΔGf° = -649.913 + 26.667x10^{-3}TlnT - 14.031x10^{-6}T^{2} + 418.812T^{-1} - 27.728x10^{-3}T$
1185-1200 K: $ΔHf° = -671.075 + 7.617x10^{-3}T - 0.031x10^{-6}T^{2} + 944.271T^{-1}$
$ΔGf° = -671.075 - 7.617x10^{-3}TlnT + 0.031x10^{-6}T^{2} + 472.136T^{-1} + 216.075x10^{-3}T$

Source: Data from Bennington (33).

NaH(c)
Sodium Hydride
[Formation: $Na(c,l) + 0.5H_2(g) = NaH(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.698	9.564	9.564	0	-13.450	-7.983	5.851
300	8.732	9.618	9.565	.016	-13.453	-7.948	5.790
371*	9.739	11.595	9.765	.679	-13.539	-6.635	3.909
371	9.739	11.595	9.765	.679	-14.161	-6.635	3.909
400	10.150	12.343	9.926	.967	-14.193	-6.046	3.303
500	11.270	14.734	10.654	2.040	-14.210	-4.005	1.751
600	12.120	16.868	11.515	3.212	-14.109	-1.972	.718
700	12.840	18.792	12.419	4.461	-13.917	.036	-.011
800	13.400	20.545	13.326	5.775	-13.651	2.013	-.550

*Data above 350 K estimated.

Phase change: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 8.874 + 6.162\text{x}10^{-3}T - 1.790\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 8.874\text{x}10^{-3}T + 3.081\text{x}10^{-6}T^{2} + 1.790\text{x}10^{2}T^{-1} - 3.520$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -14.425 + 1.695\text{x}10^{-3}T - 1.786\text{x}10^{-6}T^{2} + 187.250T^{-1}$
$\Delta Gf° = -14.425 - 1.695\text{x}10^{-3}T\ln T + 1.786\text{x}10^{-6}T^{2} + 93.625T^{-1} + 29.678\text{x}10^{-3}T$
371-800 K: $\Delta Hf° = -14.813 - 1.358\text{x}10^{-3}T + 2.964\text{x}10^{-6}T^{2} + 278.150T^{-1}$
$\Delta Gf° = -14.813 + 1.358\text{x}10^{-3}T\ln T - 2.964\text{x}10^{-6}T^{2} + 139.075T^{-1} + 14.094\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127) who estimated all above 350 K.

NaH(g)
Sodium Hydride (ideal gas)
[Formation: Na(c,l,g) + $0.5H_2(g)$ = NaH(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.241	45.000	45.000	0	31.130	26.032	-19.082
300	7.246	45.045	45.002	.013	31.125	26.001	-18.941
371	7.490	46.609	45.163	.536	30.899	24.812	-14.616
371	7.490	46.609	45.163	.536	30.277	24.812	-14.616
400	7.589	47.176	45.288	.755	30.175	24.389	-13.325
500	7.911	48.905	45.845	1.530	29.860	22.980	-10.044
600	8.172	50.372	46.480	2.335	29.594	21.629	-7.878
700	8.377	51.647	47.128	3.163	29.365	20.320	-6.344
800	8.537	52.777	47.766	4.009	29.163	19.042	-5.202
900	8.664	53.790	48.380	4.869	28.978	17.788	-4.319
1000	8.767	54.708	48.967	5.741	28.800	16.555	-3.618
1100	8.853	55.548	49.528	6.622	28.622	15.337	-3.047
1177	8.909	56.148	49.941	7.306	28.483	14.417	-2.677
1177	8.909	56.148	49.941	7.306	5.198	14.417	-2.677
1200	8.926	56.321	50.062	7.511	5.202	14.594	-2.658
1300	8.989	57.038	50.571	8.407	5.229	15.379	-2.585
1400	9.044	57.707	51.058	9.309	5.257	16.157	-2.522
1500	9.094	58.332	51.522	10.215	5.282	16.933	-2.467
1600	9.139	58.921	51.967	11.127	5.308	17.709	-2.419
1700	9.181	59.476	52.392	12.043	5.334	18.483	-2.376
1800	9.220	60.002	52.800	12.963	5.358	19.255	-2.338
1900	9.257	60.501	53.192	13.887	5.382	20.029	-2.304
2000	9.292	60.977	53.569	14.815	5.406	20.799	-2.273

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.851 + 0.882\times10^{-3}T - 0.776\times10^{5}T^{-2}$
$H°-H°_{298} = 7.851\times10^{-3}T + 0.441\times10^{-6}T^{2} + 0.776\times10^{2}T^{-1} - 2.640$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = 31.035 + 0.672\times10^{-3}T - 4.426\times10^{-6}T^{2} + 85.850T^{-1}$
$\Delta Gf° = 31.035 - 0.672\times10^{-3}T\ln T + 4.426\times10^{-6}T^{2} + 42.925T^{-1} - 14.754\times10^{-3}T$
371-1177 K: $\Delta Hf° = 30.647 - 2.381\times10^{-3}T + 0.323\times10^{-6}T^{2} + 176.750T^{-1}$
$\Delta Gf° = 30.647 + 2.381\times10^{-3}T\ln T - 0.323\times10^{-6}T^{2} + 88.375T^{-1} - 30.338\times10^{-3}T$
1177-2000 K: $\Delta Hf° = 5.184 - 0.344\times10^{-3}T + 0.227\times10^{-6}T^{2} + 74.850T^{-1}$
$\Delta Gf° = 5.184 + 0.344\times10^{-3}T\ln T - 0.227\times10^{-6}T^{2} + 37.425T^{-1} + 5.622\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127).

$NaHCO_3(c)$
Sodium Hydrogen Carbonate, Nahcolite
[Formation: $Na(c,l) + 0.5H_2(g) + C(c) + 1.5O_2(g) = NaHCO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	20.983	24.400	24.400	0	-226.805	-203.436	149.120
300	21.047	24.530	24.400	.039	-226.808	-203.290	148.095
371	23.489	29.251	24.883	1.620	-226.894	-197.713	116.468
371	23.489	29.251	24.883	1.620	-227.516	-197.713	116.468
400	24.486	31.056	25.266	2.316	-227.531	-195.382	106.751
500	27.925	36.889	27.017	4.936	-227.415	-187.353	81.891

Phase change: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp° = 10.946 + 33.996\times10^{-3}T - 0.088\times10^{5}T^{-2}$
$H°-H°_{298} = 10.946\times10^{-3}T + 16.998\times10^{-6}T^{2} + 0.088\times10^{2}T^{-1} - 4.804$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -223.841 - 10.596\times10^{-3}T + 10.610\times10^{-6}T^{2} - 223.050T^{-1}$
$\Delta Gf° = -223.841 + 10.596\times10^{-3}T\ln T - 10.610\times10^{-6}T^{2} - 111.525T^{-1} + 12.485\times10^{-3}T$
371-500 K: $\Delta Hf° = -224.229 - 13.649\times10^{-3}T + 15.360\times10^{-6}T^{2} - 132.150T^{-1}$
$\Delta Gf° = -224.229 + 13.649\times10^{-3}T\ln T - 15.360\times10^{-6}T^{2} - 66.075T^{-1} - 3.099\times10^{-3}T$

Source: Data from Chang (74).

$NaLiSO_4$(c,l)
Sodium Lithium Sulfate
[Reaction: Na(c,l,g) + Li(c,l) + $0.5S_2$(g) + $2O_2$(g) = $NaLiSO_4$(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	29.900	31.550	31.550	0	-353.385	-319.704	234.347
300	29.981	31.735	31.552	.055	-353.386	-319.495	232.749
371	33.246	38.428	32.238	2.297	-353.366	-311.474	183.482
371	33.246	38.428	32.238	2.297	-353.988	-311.474	183.482
400	34.579	40.980	32.780	3.280	-353.945	-308.152	168.364
453.7	37.273	45.491	34.018	5.205	-353.785	-302.013	145.480
453.7	37.273	45.491	34.018	5.205	-354.502	-302.013	145.480
500	39.596	49.226	35.256	6.985	-354.275	-296.666	129.671
600	45.031	56.919	38.231	11.213	-353.414	-285.215	103.888
700	50.880	64.295	41.431	16.005	-352.015	-273.954	85.531
792	56.630	70.923	44.473	20.948	-350.216	-263.804	72.795
792	55.327	77.174	44.473	25.899	-345.265	-263.804	72.795
800	54.725	77.725	44.801	26.339	-345.100	-262.981	71.842
888	49.132	83.136	48.343	30.896	-343.576	-254.034	62.521
888	51.883	84.233	48.343	31.870	-342.602	-254.034	62.521
900	51.714	84.928	48.826	32.492	-342.396	-252.838	61.397
1000	50.672	90.318	52.712	37.606	-340.759	-242.978	53.102
1100	50.294	95.124	56.353	42.648	-339.227	-233.274	46.347
1177	50.519	98.530	59.002	46.524	-338.071	-225.893	41.944
1177	50.519	98.530	59.002	46.524	-361.356	-225.893	41.944
1200	50.586	99.508	59.769	47.687	-360.964	-223.252	40.659

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
792 K, α - β transition point of $NaLiSO_4$; ΔH° = 4.951 kcal/mol.
888 K, melting point of $NaLiSO_4$; ΔH° = 0.974 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-792 K: $Cp^\circ = 9.940 + 57.676\text{x}10^{-3}T + 2.457\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 9.940\text{x}10^{-3}T + 28.838\text{x}10^{-6}T^2 - 2.457\text{x}10^{2}T^{-1} - 4.703$
792-888 K: $Cp^\circ = 108.330 - 66.996\text{x}10^{-3}T$
$H^\circ - H^\circ_{298} = 108.330\text{x}10^{-3}T - 33.498\text{x}10^{-6}T^2 - 38.886$
888-1200 K: $Cp^\circ = 18.519 + 19.158\text{x}10^{-3}T + 129.739\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 18.519\text{x}10^{-3}T + 9.579\text{x}10^{-6}T^2 - 129.739\text{x}10^{2}T^{-1} + 22.482$

Reaction equations (kcal/mol):

298.15-371 K: $\Delta Hr^\circ = -349.706 - 14.342\text{x}10^{-3}T + 17.556\text{x}10^{-6}T^2 - 287.250T^{-1}$
$\Delta Gr^\circ = -349.706 + 14.342\text{x}10^{-3}T\ln T - 17.556\text{x}10^{-6}T^2 - 143.625T^{-1} + 25.764\text{x}10^{-3}T$
371-453.7 K: $\Delta Hr^\circ = -350.094 - 17.395\text{x}10^{-3}T + 22.306\text{x}10^{-6}T^2 - 196.350T^{-1}$
$\Delta Gr^\circ = -350.094 + 17.395\text{x}10^{-3}T\ln T - 22.306\text{x}10^{-6}T^2 - 98.175T^{-1} + 10.181\text{x}10^{-3}T$
453.7-792 K: $\Delta Hr^\circ = -349.655 - 22.493\text{x}10^{-3}T + 27.770\text{x}10^{-6}T^2 - 182.050T^{-1}$
$\Delta Gr^\circ = -349.655 + 22.493\text{x}10^{-3}T\ln T - 27.770\text{x}10^{-6}T^2 - 91.025T^{-1} - 19.531\text{x}10^{-3}T$
792-888 K: $\Delta Hr^\circ = -383.838 + 75.898\text{x}10^{-3}T - 34.566\text{x}10^{-6}T^2 + 63.650T^{-1}$
$\Delta Gr^\circ = -383.838 - 75.898\text{x}10^{-3}T\ln T + 34.566\text{x}10^{-6}T^2 + 31.825T^{-1} + 630.774\text{x}10^{-3}T$
888-1177 K: $\Delta Hr^\circ = -322.469 - 13.914\text{x}10^{-3}T + 8.511\text{x}10^{-6}T^2 - 12910.250T^{-1}$
$\Delta Gr^\circ = -322.469 + 13.914\text{x}10^{-3}T\ln T - 8.511\text{x}10^{-6}T^2 - 6455.125T^{-1} - 1.580\text{x}10^{-3}T$
1177-1200 K: $\Delta Hr^\circ = -347.932 - 11.877\text{x}10^{-3}T + 8.415\text{x}10^{-6}T^2 - 13012.150T^{-1}$
$\Delta Gr^\circ = -347.932 + 11.877\text{x}10^{-3}T\ln T - 8.415\text{x}10^{-6}T^2 - 6506.075T^{-1} + 34.380\text{x}10^{-3}T$

Source: Data from O'Hare (371).

$Na_2MoO_4(c,l)$
Sodium Molybdate
[Formation: $2Na(c,l,g) + Mo(c) + 2O_2(g) = Na_2MoO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	33.870	38.130	38.130	0	-350.890	-323.661	237.247
300	33.957	38.340	38.130	.063	-350.888	-323.491	235.660
371	36.479	45.875	38.907	2.585	-350.790	-317.017	186.747
371	36.479	45.875	38.907	2.585	-352.034	-317.017	186.747
400	37.509	48.659	39.514	3.658	-351.988	-314.282	171.713
500	39.726	57.280	42.228	7.526	-351.671	-304.885	133.263
600	41.458	64.681	45.369	11.587	-351.187	-295.572	107.661
700	42.961	71.186	48.600	15.810	-350.569	-286.350	89.401
718	43.217	72.280	49.181	16.585	-350.446	-284.701	86.658
718	35.406	79.523	49.181	21.785	-345.246	-284.701	86.658
800	45.326	83.878	52.509	25.095	-344.919	-277.798	75.890
866	53.310	87.784	55.047	28.350	-344.080	-272.290	68.716
866	43.648	88.361	55.047	28.850	-343.580	-272.290	68.716
900	50.764	90.178	56.339	30.455	-343.226	-269.497	65.442
915	53.903	91.043	56.901	31.240	-342.994	-268.270	64.076
915	55.534	93.207	56.901	33.220	-341.014	-268.270	64.076
962	44.891	95.724	58.739	35.580	-340.392	-264.552	60.101
962	50.910	101.047	58.739	40.700	-335.272	-264.552	60.101
1000	50.910	103.019	60.384	42.635	-334.750	-261.769	57.209
1100	50.910	107.871	64.484	47.726	-333.413	-254.537	50.571
1177	50.910	111.316	67.436	51.646	-332.413	-249.041	46.242
1177	50.910	111.316	67.436	51.646	-378.983	-249.041	46.242
1200	50.910	112.301	68.287	52.817	-378.598	-246.510	44.895
1300	50.910	116.376	71.831	57.908	-376.926	-235.567	39.602
1400	50.910	120.149	75.150	62.999	-375.288	-224.756	35.086
1500	50.910	123.661	78.268	68.090	-373.680	-214.064	31.189

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
718 K, α - β transition point of Na_2MoO_4; ΔH° = 5.200 kcal/mol.
866 K, β - γ transition point of Na_2MoO_4; ΔH° = 0.500 kcal/mol.
915 K, γ - δ transition point of Na_2MoO_4; ΔH° = 1.980 kcal/mol.
962 K, melting point of Na_2MoO_4; ΔH° = 5.120 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-718 K: $Cp° = 35.832 + 11.558\times10^{-3}T - 4.714\times10^{5}T^{-2}$
$H° - H°_{298} = 35.832\times10^{-3}T + 5.779\times10^{-6}T^{2} + 4.714\times10^{2}T^{-1} - 12.778$
718-866 K: $Cp° = -51.456 + 120.978\times10^{-3}T$
$H° - H°_{298} = -51.456\times10^{-3}T + 60.489\times10^{-6}T^{2} + 27.547$
866-915 K: $Cp° = -137.592 + 209.284\times10^{-3}T$
$H° - H°_{298} = -137.592\times10^{-3}T + 104.642\times10^{-6}T^{2} + 69.528$
915-962 K: $Cp° = 262.730 - 226.446\times10^{-3}T$
$H° - H°_{298} = 262.730\times10^{-3}T - 113.223\times10^{-6}T^{2} - 112.385$
962-1500 K: $Cp° = 50.910$
$H° - H°_{298} = 50.910\times10^{-3}T - 8.275$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -354.568 + 9.093\times10^{-3}T - 5.728\times10^{-6}T^{2} + 440.200T^{-1}$
$\Delta Gf° = -354.568 - 9.093\times10^{-3}T\ln T + 5.728\times10^{-6}T^{2} + 220.100T^{-1} + 151.288\times10^{-3}T$
371-718 K: $\Delta Hf° = -355.345 + 2.987\times10^{-3}T + 3.772\times10^{-6}T^{2} + 622.000T^{-1}$
$\Delta Gf° = -355.345 - 2.987\times10^{-3}T\ln T - 3.772\times10^{-6}T^{2} + 311.000T^{-1} + 120.120\times10^{-3}T$
718-866 K: $\Delta Hf° = -315.020 - 84.301\times10^{-3}T + 58.482\times10^{-6}T^{2} + 150.600T^{-1}$
$\Delta Gf° = -315.020 + 84.301\times10^{-3}T\ln T - 58.482\times10^{-6}T^{2} + 75.300T^{-1} - 470.351\times10^{-3}T$
866-915 K: $\Delta Hf° = -273.039 - 170.437\times10^{-3}T + 102.635\times10^{-6}T^{2} + 150.600T^{-1}$
$\Delta Gf° = -273.039 + 170.437\times10^{-3}T\ln T - 102.635\times10^{-6}T^{2} + 75.300T^{-1} - 1063.204\times10^{-3}T$
915-962 K: $\Delta Hf° = -454.951 + 229.885\times10^{-3}T - 115.230\times10^{-6}T^{2} + 150.600T^{-1}$
$\Delta Gf° = -454.951 - 229.885\times10^{-3}T\ln T + 115.230\times10^{-6}T^{2} + 75.300T^{-1} + 1666.025\times10^{-3}T$
962-1177 K: $\Delta Hf° = -350.842 + 18.065\times10^{-3}T - 2.007\times10^{-6}T^{2} + 150.600T^{-1}$
$\Delta Gf° = -350.842 - 18.065\times10^{-3}T\ln T + 2.007\times10^{-6}T^{2} + 75.300T^{-1} + 211.729\times10^{-3}T$
1177-1500 K: $\Delta Hf° = -401.768 + 22.139\times10^{-3}T - 2.199\times10^{-6}T^{2} - 53.200T^{-1}$
$\Delta Gf° = -401.768 - 22.139\times10^{-3}T\ln T + 2.199\times10^{-6}T^{2} - 26.600T^{-1} + 283.650\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Weller (522). High-temperature data based on Denielou (117).

$NaN_3(c)$
Sodium Azide
[Formation: $Na(c,l) + 1.5N_2(g) = NaN_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	18.310	23.150	23.150	0	5.190	22.424	-16.437
300	18.340	23.260	23.150	.034	5.193	22.532	-16.415
371	19.753	27.322	23.573	1.391	5.305	26.621	-15.682
371	19.753	27.322	23.573	1.391	4.683	26.621	-15.682
400	20.330	28.830	23.900	1.972	4.741	28.334	-15.481
500	21.530	33.510	25.366	4.072	5.046	34.201	-14.949
600	22.250	37.500	27.063	6.262	5.445	39.995	-14.568

Phase change: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 20.457 + 4.504\times10^{-3}T - 3.102\times10^{5}T^{-2}$
$H°-H°_{298} = 20.457\times10^{-3}T + 2.252\times10^{-6}T^{2} + 3.102\times10^{2}T^{-1} - 7.340$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = 2.396 + 6.731\times10^{-3}T - 3.289\times10^{-6}T^{2} + 322.050T^{-1}$
$\Delta Gf° = 2.396 - 6.731\times10^{-3}T\ln T + 3.289\times10^{-6}T^{2} + 161.025T^{-1} + 102.731\times10^{-3}T$
371-600 K: $\Delta Hf° = 2.007 + 3.678\times10^{-3}T + 1.460\times10^{-6}T^{2} + 412.950T^{-1}$
$\Delta Gf° = 2.007 - 3.678\times10^{-3}T\ln T - 1.460\times10^{-6}T^{2} + 206.475T^{-1} + 87.147\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Carling (71). High-temperature data based on Fritzer (162).

$NaNO_2(c,l)$
Sodium Nitrite
[Formation: $Na(c,l) + 0.5N_2(g) + O_2(g) = NaNO_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	22.200	24.800	24.800	0	-85.720	-68.013	49.855
300	22.203	24.937	24.800	.041	-85.711	-67.903	49.467
371	26.761	29.672	25.300	1.622	-85.382	-63.728	37.541
371	26.761	29.672	25.300	1.622	-86.004	-63.728	37.541
400	28.623	31.756	25.694	2.425	-85.729	-61.997	33.873
437	37.893	34.655	26.325	3.640	-85.189	-59.824	29.918
437	32.053	35.616	26.325	4.060	-84.769	-59.824	29.918
500	31.818	39.835	27.769	6.033	-83.945	-56.285	24.602
554	37.500	43.338	29.114	7.880	-83.085	-53.340	21.042
554	28.663	49.367	29.114	11.220	-79.745	-53.340	21.042
600	28.427	51.646	30.756	12.534	-79.276	-51.166	18.637
700	26.820	55.926	34.056	15.309	-78.349	-46.557	14.536

*Heat capacity at 298 K estimated.

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
437 K, α - β transition point of $NaNO_2$; ΔH° = 0.420 kcal/mol.
554 K, melting point of $NaNO_2$; ΔH° = 3.340 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-437 K: $Cp° = -142.012 + 342.220x10^{-3}T + 55.290x10^{5}T^{-2}$
$H°-H°_{298} = -142.012x10^{-3}T + 171.110x10^{-6}T^{2} - 55.290x10^{2}T^{-1} + 45.675$
437-554 K: $Cp° = -97.881 + 185.936x10^{-3}T + 92.963x10^{5}T^{-2}$
$H°-H°_{298} = -97.881x10^{-3}T + 92.968x10^{-6}T^{2} - 92.963x10^{2}T^{-1} + 50.353$
554-700 K: $Cp° = 64.475 - 43.094x10^{-3}T - 36.637x10^{5}T^{-2}$
$H°-H°_{298} = 64.475x10^{-3}T - 21.547x10^{-6}T^{2} + 36.637x10^{2}T^{-1} - 24.499$

Formation equations (kcal/mol):

298.15-371 K: $ΔHf° = -35.117 - 156.452x10^{-3}T + 165.655x10^{-6}T^{2} - 5570.250T^{-1}$
$ΔGf° = -35.117 + 156.452x10^{-3}TlnT - 165.655x10^{-6}T^{2} - 2785.125T^{-1} - 921.012x10^{-3}T$
371-437 K: $ΔHf° = -35.505 - 159.505x10^{-3}T + 170.404x10^{-6}T^{2} - 5479.350T^{-1}$
$ΔGf° = -35.505 + 159.505x10^{-3}TlnT - 170.404x10^{-6}T^{2} - 2739.675T^{-1} - 936.596x10^{-3}T$
437-554 K: $ΔHf° = -30.827 - 115.373x10^{-3}T + 92.263x10^{-6}T^{2} - 9246.650T^{-1}$
$ΔGf° = -30.827 + 115.373x10^{-3}TlnT - 92.263x10^{-6}T^{2} - 4623.325T^{-1} - 703.272x10^{-3}T$
554-700 K: $ΔHf° = -105.679 + 46.983x10^{-3}T - 22.253x10^{-6}T^{2} + 3713.350T^{-1}$
$ΔGf° = -105.679 - 46.983x10^{-3}TlnT + 22.253x10^{-6}T^{2} + 1856.675T^{-1} + 372.915x10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (516). Heat capacity at 298 K estimated. High-temperature data based on Janz (217).

$NaNO_3$(c,l)
Sodium Nitrate
[Formation: Na(c,l) + $0.5N_2$(g) + $1.5O_2$(g) = $NaNO_3$(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	22.000	27.850	27.850	0	-111.820	-87.717	64.298
300	22.100	27.990	27.857	.040	-111.818	-87.569	63.793
371	25.295	32.957	28.355	1.708	-111.654	-81.842	48.211
371	25.295	32.957	28.355	1.708	-112.276	-81.842	48.211
400	26.600	34.910	28.760	2.460	-112.156	-79.467	43.418
500	35.880	41.620	30.660	5.480	-111.324	-71.377	31.198
550	90.990	46.780	31.853	8.210	-109.696	-67.437	26.797
550	36.000	46.780	31.853	8.210	-109.696	-67.437	26.797
583	36.000	48.880	32.755	9.400	-109.237	-64.914	24.334
583	33.400	55.070	32.755	13.010	-105.627	-64.914	24.334
600	33.400	56.030	33.397	13.580	-105.435	-63.726	23.212
700	33.400	61.180	37.009	16.920	-104.331	-56.864	17.754
800	33.400	65.640	40.315	20.260	-103.255	-50.158	13.702

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
550 K, second order transition point of $NaNO_3$; ΔH° = 0 kcal/mol.
583 K, melting point of $NaNO_3$; ΔH° = 3.610 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = -67.113 + 195.864\times10^{-3}T + 27.305\times10^{5}T^{-2}$
$H°-H°_{298} = -67.113\times10^{-3}T + 97.932\times10^{-6}T^{2} - 27.305\times10^{2}T^{-1} + 20.462$
550-583 K: $Cp° = 36.000$
$H°-H°_{298} = 36.000\times10^{-3}T - 11.590$
583-800 K: $Cp° = 33.400$
$H°-H°_{298} = 33.400\times10^{-3}T - 6.462$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -85.253 - 85.167\times10^{-3}T + 92.225\times10^{-6}T^{2} - 2794.350T^{-1}$
$\Delta Gf° = -85.253 + 85.167\times10^{-3}T\ln T - 92.225\times10^{-6}T^{2} - 1397.175T^{-1} - 450.301\times10^{-3}T$
371-550 K: $\Delta Hf° = -85.641 - 88.220\times10^{-3}T + 96.975\times10^{-6}T^{2} - 2703.450T^{-1}$
$\Delta Gf° = -85.641 + 88.220\times10^{-3}T\ln T - 96.975\times10^{-6}T^{2} - 1351.725T^{-1} - 465.885\times10^{-3}T$
550-583 K: $\Delta Hf° = -117.694 + 14.892\times10^{-3}T - 0.957\times10^{-6}T^{2} + 27.050T^{-1}$
$\Delta Gf° = -117.694 - 14.892\times10^{-3}T\ln T + 0.957\times10^{-6}T^{2} + 13.525T^{-1} + 184.651\times10^{-3}T$
583-800 K: $\Delta Hf° = -112.568 + 12.293\times10^{-3}T - 0.957\times10^{-6}T^{2} + 27.050T^{-1}$
$\Delta Gf° = -112.568 - 12.293\times10^{-3}T\ln T + 0.957\times10^{-6}T^{2} + 13.525T^{-1} + 159.302\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Carling (69). High-temperature data based on Carling (69) and Rogers (430).

NaOH(c,l)
Sodium Hydroxide
[Formation: Na(c,l,g) + $0.5O_2$(g) + $0.5H_2$(g) = NaOH(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	14.228	15.403	15.403	0	-101.723	-90.691	66.478
300	14.260	15.491	15.404	.026	-101.722	-90.622	66.018
371	15.155	18.621	15.728	1.073	-101.675	-88.001	51.839
371	15.155	18.621	15.728	1.073	-102.297	-88.001	51.839
400	15.520	19.775	15.980	1.518	-102.276	-86.884	47.471
500	17.963	23.464	17.112	3.176	-102.074	-83.054	36.302
572	20.300	26.100	18.131	4.558	-101.735	-80.369	30.707
572	20.560	29.107	18.131	6.278	-100.015	-80.369	30.707
596	20.560	29.893	18.532	6.771	-99.870	-79.513	29.157
596	20.576	32.544	18.532	8.351	-98.290	-79.513	29.157
600	20.570	32.682	18.627	8.433	-98.266	-79.387	28.916
700	20.430	35.843	20.867	10.483	-97.661	-76.290	23.819
800	20.290	38.562	22.913	12.519	-97.073	-73.278	20.018
900	20.150	40.943	24.786	14.541	-96.503	-70.337	17.080
1000	20.010	43.059	26.510	16.549	-95.958	-67.460	14.743
1100	19.870	44.960	28.103	18.543	-95.442	-64.636	12.842
1177	19.762	46.301	29.250	20.069	-95.065	-62.489	11.603
1177	19.762	46.301	29.250	20.069	-118.350	-62.489	11.603
1200	19.730	46.683	29.580	20.523	-118.195	-61.401	11.182
1300	19.590	48.256	30.957	22.489	-117.526	-56.692	9.531
1400	19.450	49.703	32.245	24.441	-116.881	-52.038	8.123
1500	19.310	51.040	33.454	26.379	-116.259	-47.429	6.910
1600	19.170	52.282	34.593	28.303	-115.659	-42.861	5.854
1700	19.030	53.440	35.668	30.213	-115.080	-38.328	4.927
1800	18.910	54.524	36.685	32.110	-114.522	-33.829	4.107

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
572 K, α - β transition point of NaOH; ΔH° = 1.720 kcal/mol.
596 K, melting point of NaOH; ΔH° = 1.580 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1830 K, boiling point to monomeric NaOH; ΔH° = 41.9 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-572 K: $Cp^\circ = -2.064 + 36.530\times10^{-3}T + 4.801\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = -2.064\times10^{-3}T + 18.265\times10^{-6}T^2 - 4.801\times10^{2}T^{-1} + 0.602$
572-596 K: $Cp^\circ = 20.561$
$H^\circ - H^\circ_{298} = 20.561\times10^{-3}T - 5.483$
596-1800 K: $Cp^\circ = 21.401 - 1.394\times10^{-3}T + 0.021\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 21.401\times10^{-3}T - 0.697\times10^{-6}T^2 - 0.021\times10^{2}T^{-1} - 4.153$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -97.400 - 12.858\times10^{-3}T + 13.146\times10^{-6}T^2 - 494.450T^{-1}$
$\Delta Gf^\circ = -97.400 + 12.858\times10^{-3}T\ln T - 13.146\times10^{-6}T^2 - 247.225T^{-1} - 44.059\times10^{-3}T$
371-572 K: $\Delta Hf^\circ = -97.788 - 15.911\times10^{-3}T + 17.896\times10^{-6}T^2 - 403.550T^{-1}$
$\Delta Gf^\circ = -97.788 + 15.911\times10^{-3}T\ln T - 17.896\times10^{-6}T^2 - 201.775T^{-1} - 59.643\times10^{-3}T$
572-596 K: $\Delta Hf^\circ = -103.873 + 6.714\times10^{-3}T - 0.369\times10^{-6}T^2 + 76.550T^{-1}$
$\Delta Gf^\circ = -103.873 - 6.714\times10^{-3}T\ln T + 0.369\times10^{-6}T^2 + 38.275T^{-1} + 83.463\times10^{-3}T$
596-1177 K: $\Delta Hf^\circ = -102.542 + 7.554\times10^{-3}T - 1.066\times10^{-6}T^2 + 74.450T^{-1}$
$\Delta Gf^\circ = -102.542 - 7.554\times10^{-3}T\ln T + 1.066\times10^{-6}T^2 + 37.225T^{-1} + 86.186\times10^{-3}T$
1177-1800 K: $\Delta Hf^\circ = -128.005 + 9.591\times10^{-3}T - 1.162\times10^{-6}T^2 - 27.450T^{-1}$
$\Delta Gf^\circ = -128.005 - 9.591\times10^{-3}T\ln T + 1.162\times10^{-6}T^2 - 13.725T^{-1} + 122.147\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from Chase (81).

$NaOH(g)$
Sodium Hydroxide (ideal gas)
[Formation: $Na(c,l,g) + 0.5O_2(g) + 0.5H_2(g) = NaOH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.561	54.572	54.572	0	-47.300	-47.946	35.145
300	11.575	54.644	54.574	.021	-47.304	-47.950	34.931
371	11.955	57.150	54.832	.860	-47.465	-48.086	28.326
371	11.955	57.150	54.832	.860	-48.087	-48.086	28.326
400	12.110	58.056	55.034	1.209	-48.162	-48.083	26.271
500	12.389	60.791	55.921	2.435	-48.392	-48.035	20.996
600	12.563	63.067	56.929	3.683	-48.593	-47.945	17.464
700	12.698	65.014	57.947	4.947	-48.775	-47.823	14.931
800	12.822	66.717	58.938	6.223	-48.945	-47.675	13.024
900	12.944	68.235	59.889	7.511	-49.110	-47.507	11.536
1000	13.067	69.605	60.794	8.811	-49.272	-47.321	10.342
1100	13.190	70.856	61.652	10.124	-49.438	-47.118	9.361
1177	13.282	71.752	62.284	11.143	-49.568	-46.947	8.717
1177	13.282	71.752	62.284	11.143	-72.853	-46.947	8.717
1200	13.310	72.009	62.468	11.449	-72.846	-46.443	8.458
1300	13.425	73.079	63.244	12.786	-72.806	-44.242	7.438
1400	13.534	74.078	63.982	14.134	-72.765	-42.047	6.564
1500	13.635	75.015	64.686	15.493	-72.722	-39.855	5.807
1600	13.729	75.898	65.360	16.861	-72.678	-37.666	5.145
1700	13.816	76.733	66.005	18.238	-72.632	-35.479	4.561
1800	13.895	77.525	66.623	19.624	-72.586	-33.294	4.042
1900	13.968	78.278	67.216	21.017	-72.540	-31.112	3.579
2000	14.034	78.996	67.788	22.417	-72.493	-28.932	3.162

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.219 + 0.956x10^{-3}T - 0.839x10^{5}T^{-2}$
$H°- H°_{298} = 12.219x10^{-3}T + 0.478x10^{-6}T^{2} + 0.839x10^{2}T^{-1} - 3.967$

Formation equations (kcal/mol):

298.15-371 K: $ΔHf° = -47.546 + 1.425x10^{-3}T - 4.641x10^{-6}T^{2} + 69.550T^{-1}$
$ΔGf° = -47.546 - 1.425x10^{-3}TlnT + 4.641x10^{-6}T^{2} + 34.775T^{-1} + 5.000x10^{-3}T$
371-1177 K: $ΔHf° = -47.934 - 1.628x10^{-3}T + 0.109x10^{-6}T^{2} + 160.450T^{-1}$
$ΔGf° = -47.934 + 1.628x10^{-3}TlnT - 0.109x10^{-6}T^{2} + 80.225T^{-1} - 10.584x10^{-3}T$
1177-2000 K: $ΔHf° = -73.397 + 0.409x10^{-3}T + 0.013x10^{-6}T^{2} + 58.550T^{-1}$
$ΔGf° = -73.397 - 0.409x10^{-3}TlnT - 0.013x10^{-6}T^{2} + 29.275T^{-1} + 25.377x10^{-3}T$

Source: Data from Chase (81) who estimated some molecular constants.

$(NaOH)_2(g)$
Dimeric Sodium Hydroxide (ideal gas)
[Formation: $2Na(c,l,g) + O_2(g) + H_2(g) = (NaOH)_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	18.949	73.442	73.442	0	-145.200	-135.848	99.578
300	18.985	73.559	73.442	.035	-145.215	-135.789	98.921
371	20.249	77.729	73.873	1.430	-145.820	-133.493	78.637
371	20.249	77.729	73.873	1.430	-147.064	-133.493	78.637
400	20.765	79.272	74.210	2.025	-147.317	-132.422	72.351
500	22.248	84.070	75.714	4.178	-148.076	-128.607	56.213
600	23.434	88.236	77.461	6.465	-148.686	-124.653	45.404
700	24.381	91.922	79.269	8.857	-149.186	-120.609	37.655
800	25.157	95.230	81.061	11.335	-149.602	-116.497	31.825
900	25.813	98.232	82.805	13.884	-149.958	-112.337	27.279
1000	26.381	100.981	84.486	16.495	-150.272	-108.139	23.633
1100	26.881	103.520	86.104	19.158	-150.566	-103.915	20.646
1177	27.222	105.350	87.303	21.242	-150.780	-100.633	18.686
1177	27.222	105.350	87.303	21.242	-197.350	-100.633	18.686
1200	27.324	105.878	87.654	21.869	-197.321	-98.747	17.984
1300	27.720	108.081	89.141	24.622	-197.162	-90.533	15.220
1400	28.073	110.148	90.568	27.412	-196.986	-82.339	12.853
1500	28.386	112.096	91.939	30.235	-196.794	-74.160	10.805
1600	28.671	113.938	93.258	33.088	-196.589	-65.992	9.014
1700	28.924	115.683	94.525	35.968	-196.372	-57.834	7.435
1800	29.151	117.343	95.747	38.872	-196.147	-49.692	6.033
1900	29.355	118.925	96.926	41.798	-195.915	-41.561	4.781
2000	29.538	120.435	98.064	44.742	-195.679	-33.443	3.654

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.912 + 4.416\times10^{-3}T - 3.804\times10^{5}T^{-2}$
$H° - H°_{298} = 21.912\times10^{-3}T + 2.208\times10^{-6}T^{2} + 3.804\times10^{2}T^{-1} - 8.005$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -145.762 + 0.324\times10^{-3}T - 8.030\times10^{-6}T^{2} + 351.700T^{-1}$
$\Delta Gf° = -145.762 - 0.324\times10^{-3}T\ln T + 8.030\times10^{-6}T^{2} + 175.850T^{-1} + 30.726\times10^{-3}T$
371-1177 K: $\Delta Hf° = -146.539 - 5.782\times10^{-3}T + 1.470\times10^{-6}T^{2} + 533.500T^{-1}$
$\Delta Gf° = -146.539 + 5.782\times10^{-3}T\ln T - 1.470\times10^{-6}T^{2} + 266.750T^{-1} - 0.442\times10^{-3}T$
1177-2000 K: $\Delta Hf° = -197.465 - 1.708\times10^{-3}T + 1.278\times10^{-6}T^{2} + 329.700T^{-1}$
$\Delta Gf° = -197.465 + 1.708\times10^{-3}T\ln T - 1.278\times10^{-6}T^{2} + 164.850T^{-1} + 71.479\times10^{-3}T$

Source: Data from Chase (81) who estimated molecular constants.

$Na_2SO_4(c,l)$
Sodium Sulfate
[Reaction: $2Na(c,l,g) + 0.5S_2(g) + 2O_2(g) = Na_2SO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	30.627	35.754	35.754	0	-347.051	-313.031	229.455
300	30.711	35.944	35.754	.057	-347.051	-312.818	227.885
371	33.529	42.773	36.458	2.343	-347.057	-304.716	179.501
371	33.529	42.773	36.458	2.343	-348.301	-304.716	179.501
400	34.680	45.340	37.010	3.332	-348.283	-301.309	164.626
458	36.647	50.169	38.374	5.402	-348.158	-294.503	140.530
458	36.647	50.302	38.374	5.463	-348.097	-294.503	140.530
500	37.980	53.575	39.515	7.030	-347.943	-289.595	126.580
514	38.411	54.630	39.911	7.565	-347.879	-287.962	122.438
514	40.806	59.726	39.911	10.185	-345.259	-287.962	122.438
600	41.905	66.121	43.231	13.734	-344.615	-278.433	101.418
700	43.270	72.682	46.981	17.991	-343.756	-267.472	83.507
800	44.760	78.556	50.566	22.392	-342.777	-256.639	70.110
900	46.330	83.919	53.978	26.947	-341.670	-245.937	59.721
1000	47.875	88.880	57.223	31.657	-340.437	-235.365	51.438
1100	49.410	93.515	60.313	36.522	-339.090	-224.923	44.687
1157	50.279	96.033	62.006	39.370	-338.259	-219.012	41.369
1157	47.092	100.960	62.006	45.070	-332.559	-219.012	41.369
1177	47.092	101.767	62.675	46.012	-332.331	-217.052	40.303
1177	47.092	101.767	62.675	46.012	-378.901	-217.052	40.303
1200	47.092	102.678	63.438	47.088	-378.552	-213.903	38.957
1300	47.092	106.448	66.604	51.797	-377.002	-200.242	33.663
1400	47.092	109.938	69.577	56.506	-375.474	-186.705	29.146
1500	47.092	113.187	72.377	61.215	-373.961	-173.278	25.246
1600	47.092	116.226	75.023	65.925	-372.464	-159.946	21.847
1700	47.092	119.081	77.532	70.634	-370.983	-146.709	18.860
1800	47.092	121.773	79.916	75.343	-369.516	-133.558	16.216
1900	47.092	124.319	82.186	80.052	-368.064	-120.489	13.859
2000	47.092	126.734	84.354	84.761	-366.626	-107.495	11.746

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
458 K, V - IV transition point of Na_2SO_4; ΔH° = 0.061 kcal/mol.
514 K, IV - I transition point of Na_2SO_4; ΔH° = 2.620 kcal/mol.
1157 K, melting point of Na_2SO_4; ΔH° = 5.700 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-458 K: $Cp° = 19.722 + 37.220\times10^{-3}T$
$H°-H°_{298} = 19.722\times10^{-3}T + 18.610\times10^{-6}T^2 - 7.534$
458-514 K: $Cp° = 21.832 + 32.312\times10^{-3}T$
$H°-H°_{298} = 21.832\times10^{-3}T + 16.156\times10^{-6}T^2 - 7.925$
514-1157 K: $Cp° = 30.530 + 16.954\times10^{-3}T + 4.126\times10^{5}T^{-2}$
$H°-H°_{298} = 30.530\times10^{-3}T + 8.477\times10^{-6}T^2 - 4.126\times10^{2}T^{-1} - 6.944$
1157-2000 K: $Cp° = 47.092$
$H°-H°_{298} = 47.092\times10^{-3}T - 9.415$

Reaction equations (kcal/mol):

298.15-371 K: $\Delta Hr° = -345.325 - 6.812\times10^{-3}T + 8.128\times10^{-6}T^2 - 124.550T^{-1}$
$\Delta Gr° = -345.325 + 6.812\times10^{-3}T\ln T - 8.128\times10^{-6}T^2 - 62.275T^{-1} + 72.630\times10^{-3}T$
371-458 K: $\Delta Hr° = -346.101 - 12.917\times10^{-3}T + 17.628\times10^{-6}T^2 + 57.250T^{-1}$
$\Delta Gr° = -346.101 + 12.917\times10^{-3}T\ln T - 17.628\times10^{-6}T^2 + 28.625T^{-1} + 41.463\times10^{-3}T$
458-514 K: $\Delta Hr° = -346.492 - 10.807\times10^{-3}T + 15.174\times10^{-6}T^2 + 57.250T^{-1}$
$\Delta Gr° = -346.492 + 10.807\times10^{-3}T\ln T - 15.174\times10^{-6}T^2 + 28.625T^{-1} + 54.119\times10^{-3}T$
514-1157 K: $\Delta Hr° = -345.511 - 2.109\times10^{-3}T + 7.495\times10^{-6}T^2 - 355.350T^{-1}$
$\Delta Gr° = -345.511 + 2.109\times10^{-3}T\ln T - 7.495\times10^{-6}T^2 - 177.675T^{-1} + 103.340\times10^{-3}T$
1157-1177 K: $\Delta Hr° = -347.982 + 14.452\times10^{-3}T - 0.982\times10^{-6}T^2 + 57.250T^{-1}$
$\Delta Gr° = -347.982 - 14.452\times10^{-3}T\ln T + 0.982\times10^{-6}T^2 + 28.625T^{-1} + 212.335\times10^{-3}T$
1177-2000 K: $\Delta Hr° = -398.908 + 18.526\times10^{-3}T - 1.174\times10^{-6}T^2 - 146.550T^{-1}$
$\Delta Gr° = -398.908 - 18.526\times10^{-3}T\ln T + 1.174\times10^{-6}T^2 - 73.275T^{-1} + 284.257\times10^{-3}T$

Source: Data from Chase (80).

$Na_2SO_4(g)$
Sodium Sulfate (ideal gas)
[Reaction: $2Na(c,l,g) + 0.5S_2(g) + 2O_2(g) = Na_2SO_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	25.244	82.874	82.874	0	-262.395	-242.423	177.699
300	25.320	83.030	82.874	.047	-262.405	-242.297	176.511
371	27.769	88.690	83.455	1.942	-262.802	-237.496	139.903
371	27.769	88.690	83.455	1.942	-264.046	-237.496	139.903
400	28.769	90.818	83.913	2.762	-264.197	-235.414	128.623
500	31.119	97.507	85.979	5.764	-264.552	-228.171	99.732
600	32.726	103.332	88.397	8.961	-264.732	-220.876	80.453
700	33.845	108.465	90.904	12.293	-264.798	-213.562	66.676
800	34.644	113.040	93.390	15.720	-264.792	-206.242	56.342
900	35.229	117.156	95.806	19.215	-264.746	-198.926	48.305
1000	35.668	120.891	98.131	22.760	-264.678	-191.617	41.877
1100	36.004	124.307	100.357	26.345	-264.611	-184.315	36.620
1177	36.207	126.751	102.005	29.126	-264.561	-178.688	33.179
1177	36.207	126.751	102.005	29.126	-311.131	-178.688	33.179
1200	36.267	127.452	102.486	29.959	-311.025	-176.105	32.073
1300	36.476	130.363	104.520	33.596	-310.547	-164.877	27.718
1400	36.644	133.073	106.464	37.253	-310.070	-153.690	23.992
1500	36.782	135.606	108.323	40.924	-309.595	-142.541	20.768
1600	36.896	137.893	110.013	44.608	-309.125	-131.274	17.931
1700	36.991	140.223	111.809	48.303	-308.658	-120.326	15.469
1800	37.071	142.340	113.448	52.006	-308.197	-109.260	13.266
1900	37.140	144.346	115.022	55.716	-307.744	-98.221	11.298
2000	37.198	146.252	116.535	59.433	-307.297	-87.203	9.529

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 33.570 + 2.394\times10^{-3}T - 8.036\times10^{5}T^{-2}$
$H°-H°_{298} = 33.570\times10^{-3}T + 1.197\times10^{-6}T^{2} + 8.036\times10^{2}T^{-1} - 12.811$

Reaction equations (kcal/mol):

298.15-371 K: $\Delta Hr° = -265.945 + 7.036\times10^{-3}T - 9.285\times10^{-6}T^{2} + 679.050T^{-1}$
$\Delta Gr° = -265.945 - 7.036\times10^{-3}T\ln T + 9.285\times10^{-6}T^{2} + 339.525T^{-1} + 112.395\times10^{-3}T$
371-1177 K: $\Delta Hr° = -266.721 + 0.930\times10^{-3}T + 0.215\times10^{-6}T^{2} + 860.850T^{-1}$
$\Delta Gr° = -266.721 - 0.930\times10^{-3}T\ln T - 0.215\times10^{-6}T^{2} + 430.425T^{-1} + 81.228\times10^{-3}T$
1177-2000 K: $\Delta Hr° = -317.647 + 5.004\times10^{-3}T + 0.023\times10^{-6}T^{2} + 657.050T^{-1}$
$\Delta Gr° = -317.647 - 5.004\times10^{-3}T\ln T - 0.023\times10^{-6}T^{2} + 328.525T^{-1} + 153.149\times10^{-3}T$

Source: Data from Chase (80) who estimated some molecular constants.

$Na_2SO_4{\cdot}10H_2O(c)$
Sodium Sulfate Decahydrate
[Reaction: $2Na(c,l) + 0.5S_2(g) + 7O_2(g) + 10H_2(g) = Na_2SO_4{\cdot}10H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	124.000	141.500	141.500	0	-1049.595	-881.005	645.786
300	124.666	142.269	141.502	.230	-1049.617	-879.958	641.040
350	142.666	162.838	143.087	6.913	-1049.758	-851.658	531.793
371	150.226	171.371	144.448	9.988	-1049.581	-839.777	494.692
371	150.226	171.371	144.448	9.988	-1050.825	-839.777	494.692
400	160.666	183.064	146.822	14.497	-1050.347	-823.295	449.822
450	178.666	203.027	151.960	22.980	-1048.848	-794.995	386.097
500	196.666	222.783	158.057	32.363	-1046.484	-766.908	335.211
550	214.666	242.371	164.831	42.647	-1043.255	-739.099	293.687

Phase change: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 16.641 + 360.052 \times 10^{-3}T + 0.009 \times 10^{5}T^{-2}$
$H° - H°_{298} = 16.641 \times 10^{-3}T + 180.026 \times 10^{-6}T^{2} - 0.009 \times 10^{2}T^{-1} - 20.962$

Reaction equations (kcal/mol):

298.15-371 K: $\Delta Hr° = -1030.469 - 110.603 \times 10^{-3}T + 162.839 \times 10^{-6}T^{2} - 186.450T^{-1}$
$\Delta Gr° = -1030.469 + 110.603 \times 10^{-3}T\ln T - 162.839 \times 10^{-6}T^{2} - 93.225T^{-1} - 79.265 \times 10^{-3}T$
371-550 K: $\Delta Hr° = -1031.245 - 116.709 \times 10^{-3}T + 172.339 \times 10^{-6}T^{2} - 4.650T^{-1}$
$\Delta Gr° = -1031.245 + 116.709 \times 10^{-3}T\ln T - 172.339 \times 10^{-6}T^{2} - 2.325T^{-1} - 110.433 \times 10^{-3}T$

Source: Data from DeKock (113).

Na_2SiO_3(c,l)
Sodium Silicate
[Formation: $2Na(c,l,g) + Si(c,l) + 1.5O_2(g) = Na_2SiO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	26.740	27.210	27.210	0	-371.630	-349.151	255.932
300	26.863	27.376	27.210	.050	-371.633	-349.010	254.251
371	29.474	33.382	27.827	2.061	-371.736	-343.647	202.434
371	29.474	33.382	27.827	2.061	-372.980	-343.647	202.434
400	30.540	35.640	28.313	2.931	-373.012	-341.353	186.504
500	33.154	42.750	30.506	6.122	-372.945	-333.438	145.744
600	35.161	48.979	33.076	9.542	-372.672	-325.560	118.584
700	36.794	54.525	35.751	13.142	-372.242	-317.743	99.203
800	38.181	59.531	38.416	16.892	-371.684	-309.993	84.685
900	39.398	64.100	41.020	20.772	-371.025	-302.320	73.412
1000	40.493	68.308	43.540	24.768	-370.277	-294.716	64.409
1100	41.498	72.215	45.971	28.868	-369.465	-287.209	57.062
1177	42.218	75.048	47.782	32.092	-368.795	-281.466	52.263
1177	42.218	75.048	47.782	32.092	-415.365	-281.466	52.263
1200	42.433	75.867	48.313	33.065	-415.066	-278.857	50.786
1300	43.315	79.298	50.566	37.352	-413.705	-267.557	44.980
1362	43.835	81.325	51.917	40.054	-412.828	-260.600	41.816
1362	42.380	90.415	51.917	52.434	-400.448	-260.600	41.816
1400	42.380	91.581	52.977	54.045	-399.959	-256.704	40.073
1500	42.380	94.505	55.650	58.283	-398.683	-246.531	35.919
1600	42.380	97.240	58.164	62.521	-397.422	-236.429	32.294
1687	42.380	99.485	60.239	66.208	-396.336	-227.684	29.496
1687	42.380	99.485	60.239	66.208	-408.418	-227.684	29.496
1700	42.380	99.810	60.540	66.759	-408.248	-226.289	29.091
1800	42.380	102.232	62.789	70.997	-406.946	-215.619	26.179
1900	42.380	104.523	64.926	75.235	-405.653	-205.023	23.583
2000	42.380	106.697	66.961	79.473	-404.368	-194.503	21.254

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1362 K, melting point of Na_2SiO_3; ΔH° = 12.380 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1362 K: $Cp° = 30.472 + 10.454\times10^{-3}T - 6.093\times10^{5}T^{-2}$
$H°-H°_{298} = 30.472\times10^{-3}T + 5.227\times10^{-6}T^{2} + 6.093\times10^{2}T^{-1} - 11.593$
1362-2000 K: $Cp° = 42.380$
$H°-H°_{298} = 42.380\times10^{-3}T - 5.288$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -374.457 + 6.046\times10^{-3}T - 5.195\times10^{-6}T^{2} + 443.000T^{-1}$
$\Delta Gf° = -374.457 - 6.046\times10^{-3}T\ln T + 5.195\times10^{-6}T^{2} + 221.500T^{-1} + 115.281\times10^{-3}T$
371-1177 K: $\Delta Hf° = -375.233 - 0.060\times10^{-3}T + 4.306\times10^{-6}T^{2} + 624.800T^{-1}$
$\Delta Gf° = -375.233 + 0.060\times10^{-3}T\ln T - 4.306\times10^{-6}T^{2} + 312.400T^{-1} + 84.114\times10^{-3}T$
1177-1362 K: $\Delta Hf° = -426.159 + 4.014\times10^{-3}T + 4.114\times10^{-6}T^{2} + 421.000T^{-1}$
$\Delta Gf° = -426.159 - 4.014\times10^{-3}T\ln T - 4.114\times10^{-6}T^{2} + 210.500T^{-1} + 156.035\times10^{-3}T$
1362-1687 K: $\Delta Hf° = -419.854 + 15.922\times10^{-3}T - 1.113\times10^{-6}T^{2} - 188.300T^{-1}$
$\Delta Gf° = -419.854 - 15.922\times10^{-3}T\ln T + 1.113\times10^{-6}T^{2} - 94.150T^{-1} + 230.387\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -432.283 + 15.501\times10^{-3}T - 0.762\times10^{-6}T^{2} - 89.800T^{-1}$
$\Delta Gf° = -432.283 - 15.501\times10^{-3}T\ln T + 0.762\times10^{-6}T^{2} - 44.900T^{-1} + 235.201\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127).

$Na_2Si_2O_5(c,l)$
Sodium Disilicate
[Formation: $2Na(c,l,g) + 2Si(c,l) + 2.5O_2(g) = Na_2Si_2O_5(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	37.520	39.210	39.210	0	-589.220	-554.367	406.356
300	37.642	39.443	39.210	.070	-589.224	-554.149	403.692
371	42.038	47.918	40.077	2.909	-589.358	-545.835	321.538
371	42.038	47.918	40.077	2.909	-590.602	-545.835	321.538
400	43.834	51.149	40.764	4.154	-590.617	-542.334	296.314
500	48.577	61.467	43.895	8.786	-590.387	-530.278	231.781
600	52.002	70.643	47.601	13.825	-589.821	-518.307	188.791
700	54.455	78.854	51.491	19.154	-589.031	-506.451	158.119
800	56.205	86.246	55.381	24.692	-588.088	-494.714	135.148
900	57.439	92.942	59.189	30.378	-587.057	-483.103	117.312
951	57.986	96.123	61.085	33.321	-586.505	-477.212	109.667
951	58.000	96.228	61.085	33.421	-586.405	-477.212	109.667
980	58.000	97.970	62.151	35.103	-586.090	-473.886	105.680
980	70.000	98.123	62.151	35.253	-585.940	-473.886	105.680
1000	70.000	99.537	62.884	36.653	-585.486	-471.604	103.068
1100	70.000	106.208	66.523	43.653	-583.249	-460.341	91.460
1147	70.000	109.136	68.209	46.943	-582.213	-455.102	86.714
1147	62.430	116.547	68.209	55.443	-573.713	-455.102	86.714
1177	62.430	118.159	69.462	57.316	-573.287	-452.006	83.929
1177	62.430	118.159	69.462	57.316	-619.857	-452.006	83.929
1200	62.430	119.367	70.407	58.752	-619.440	-448.734	81.725
1300	62.430	124.364	74.368	64.995	-617.629	-434.578	73.058
1400	62.430	128.991	78.107	71.238	-615.854	-420.558	65.651
1500	62.430	133.298	81.644	77.481	-614.107	-406.695	59.255
1600	62.430	137.327	84.999	83.724	-612.386	-392.926	53.671
1687	62.430	140.633	87.784	89.155	-610.909	-380.990	49.356
1687	62.430	140.633	87.784	89.155	-635.073	-380.990	49.356
1700	62.430	141.112	88.190	89.967	-634.836	-379.025	48.726
1800	62.430	144.680	91.230	96.210	-633.027	-364.022	44.198
1900	62.430	148.056	94.133	102.453	-631.233	-349.128	40.158
2000	62.430	151.258	96.910	108.696	-629.451	-334.337	36.534

Phase changes:
371 K, melting point of Na; $\Delta H^\circ = 0.622$ kcal/mol.
951 K, α - β transition point of $Na_2Si_2O_5$; $\Delta H^\circ = 0.100$ kcal/mol.
980 K, β - γ transition point of $Na_2Si_2O_5$; $\Delta H^\circ = 0.150$ kcal/mol.
1147 K, melting point of $Na_2Si_2O_5$; $\Delta H^\circ = 8.500$ kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; $\Delta H^\circ = 23.285$ kcal/mol.
1687 K, melting point of Si; $\Delta H^\circ = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-951 K: $C_p^\circ = 42.961 + 18.422\times10^{-3}T - 9.719\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 42.961\times10^{-3}T + 9.211\times10^{-6}T^2 + 9.719\times10^{2}T^{-1} - 16.887$
951-980 K: $C_p^\circ = 58.000$
$H^\circ - H^\circ_{298} = 58.000\times10^{-3}T - 21.737$
980-1147 K: $C_p^\circ = 70.000$
$H^\circ - H^\circ_{298} = 70.000\times10^{-3}T - 33.347$
1147-2000 K: $C_p^\circ = 62.430$
$H^\circ - H^\circ_{298} = 62.430\times10^{-3}T - 16.164$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -592.934 + 5.626\times10^{-3}T - 2.064\times10^{-6}T^2 + 661.900T^{-1}$
$\Delta Gf^\circ = -592.934 - 5.626\times10^{-3}T\ln T + 2.064\times10^{-6}T^2 + 330.950T^{-1} + 157.071\times10^{-3}T$
371-951 K: $\Delta Hf^\circ = -593.710 - 0.480\times10^{-3}T + 7.436\times10^{-6}T^2 + 843.700T^{-1}$
$\Delta Gf^\circ = -593.710 + 0.480\times10^{-3}T\ln T - 7.436\times10^{-6}T^2 + 421.850T^{-1} + 125.903\times10^{-3}T$
951-980 K: $\Delta Hf^\circ = -598.560 + 14.559\times10^{-3}T - 1.775\times10^{-6}T^2 - 128.200T^{-1}$
$\Delta Gf^\circ = -598.560 - 14.559\times10^{-3}T\ln T + 1.775\times10^{-6}T^2 - 64.100T^{-1} + 225.911\times10^{-3}T$
980-1147 K: $\Delta Hf^\circ = -610.170 + 26.559\times10^{-3}T - 1.775\times10^{-6}T^2 - 128.200T^{-1}$
$\Delta Gf^\circ = -610.170 - 26.559\times10^{-3}T\ln T + 1.775\times10^{-6}T^2 - 64.100T^{-1} + 320.408\times10^{-3}T$
1147-1177 K: $\Delta Hf^\circ = -592.987 + 18.989\times10^{-3}T - 1.775\times10^{-6}T^2 - 128.200T^{-1}$
$\Delta Gf^\circ = -592.987 - 18.989\times10^{-3}T\ln T + 1.775\times10^{-6}T^2 - 64.100T^{-1} + 252.097\times10^{-3}T$
1177-1687 K: $\Delta Hf^\circ = -643.913 + 23.063\times10^{-3}T - 1.967\times10^{-6}T^2 - 332.000T^{-1}$
$\Delta Gf^\circ = -643.913 - 23.063\times10^{-3}T\ln T + 1.967\times10^{-6}T^2 - 166.000T^{-1} + 324.019\times10^{-3}T$
1687-2000 K: $\Delta Hf^\circ = -668.771 + 22.221\times10^{-3}T - 1.266\times10^{-6}T^2 - 135.000T^{-1}$
$\Delta Gf^\circ = -668.771 - 22.221\times10^{-3}T\ln T + 1.266\times10^{-6}T^2 - 67.500T^{-1} + 333.647\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from JANAF (127).

Na_2TiO_3(c,l)
Sodium Titanate

[Formation: $2Na(c,l,g) + Ti(c) + 1.5O_2(g) = Na_2TiO_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	30.030	29.060	29.060	0	-370.900	-348.132	255.184
300	30.120	29.247	29.064	.055	-370.900	-347.990	253.507
371	32.662	35.975	29.754	2.308	-370.840	-342.573	201.801
371	32.662	35.975	29.754	2.308	-372.084	-342.573	201.801
400	33.700	38.472	30.297	3.270	-372.053	-340.267	185.911
500	35.720	46.225	32.725	6.750	-371.795	-332.346	145.266
560	36.620	50.325	34.396	8.920	-371.565	-327.626	127.860
560	35.700	51.021	34.396	9.310	-371.175	-327.626	127.860
600	36.350	53.506	35.589	10.750	-371.034	-324.521	118.205
700	37.960	59.230	38.566	14.465	-370.586	-316.798	98.908
800	39.570	64.404	41.473	18.345	-370.007	-309.151	84.455
900	41.180	69.157	44.290	22.380	-369.310	-301.584	73.234
1000	42.780	73.578	46.998	26.580	-368.489	-294.098	64.274
1100	44.390	77.732	49.609	30.935	-367.568	-286.716	56.965
1156	45.292	79.958	51.025	33.447	-366.997	-282.602	53.427
1156	45.292	79.958	51.025	33.447	-368.014	-282.602	53.427
1177	45.630	80.776	51.548	34.401	-367.772	-281.052	52.186
1177	45.630	80.776	51.548	34.401	-414.342	-281.052	52.186
1200	46.000	81.663	52.117	35.455	-413.977	-270.456	50.713
1300	47.610	85.409	54.536	40.135	-412.293	-267.226	44.924
1303	47.660	85.519	54.606	40.280	-412.239	-266.889	44.764
1303	47.000	98.458	54.606	57.140	-395.379	-266.889	44.764
1400	47.000	101.833	57.762	61.700	-393.759	-257.383	40.179
1500	47.000	105.076	60.809	66.400	-392.118	-247.702	36.090
1600	47.000	108.109	63.672	71.100	-390.510	-238.127	32.526

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
560 K, α - β transition point of Na_2TiO_3; ΔH° = 0.390 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal.mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1303 K, melting point of Na_2TiO_3; ΔH° = 16.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-560 K: $Cp° = 34.385 + 7.248\times10^{-3}T - 5.724\times10^{5}T^{-2}$
$H°-H°_{298} = 34.385\times10^{-3}T + 3.624\times10^{-6}T^{2} + 5.724\times10^{2}T^{-1} - 12.494$
560-1303 K: $Cp° = 26.695 + 16.090\times10^{-3}T$
$H°-H°_{298} = 26.695\times10^{-3}T + 8.045\times10^{-6}T^{2} - 8.162$
1303-1600 K: $Cp° = 47.000$
$H°-H°_{298} = 47.000\times10^{-3}T - 4.101$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -374.899 + 10.161\times10^{-3}T - 7.570\times10^{-6}T^{2} + 489.800T^{-1}$
$\Delta Gf° = -374.899 - 10.161\times10^{-3}T\ln T + 7.570\times10^{-6}T^{2} + 244.900T^{-1} + 142.659\times10^{-3}T$
371-560 K: $\Delta Hf° = -375.676 + 4.055\times10^{-3}T + 1.930\times10^{-6}T^{2} + 671.600T^{-1}$
$\Delta Gf° = -375.676 - 4.055\times10^{-3}T\ln T - 1.930\times10^{-6}T^{2} + 335.800T^{-1} + 111.491\times10^{-3}T$
560-1156 K: $\Delta Hf° = -371.344 - 3.635\times10^{-3}T + 6.352\times10^{-6}T^{2} + 99.200T^{-1}$
$\Delta Gf° = -371.344 + 3.635\times10^{-3}T\ln T - 6.352\times10^{-6}T^{2} + 49.600T^{-1} + 58.482\times10^{-3}T$
1156-1177 K: $\Delta Hf° = -375.380 - 1.235\times10^{-3}T + 6.029\times10^{-6}T^{2} + 882.100T^{-1}$
$\Delta Gf° = -375.380 + 1.235\times10^{-3}T\ln T - 6.029\times10^{-6}T^{2} + 441.050T^{-1} + 78.234\times10^{-3}T$
1177-1303 K: $\Delta Hf° = -426.306 + 2.839\times10^{-3}T + 5.836\times10^{-6}T^{2} + 678.300T^{-1}$
$\Delta Gf° = -426.306 - 2.839\times10^{-3}T\ln T - 5.836\times10^{-6}T^{2} + 339.150T^{-1} + 150.155\times10^{-3}T$
1303-1600 K: $\Delta Hf° = -422.245 + 23.144\times10^{-3}T - 2.209\times10^{-6}T^{2} + 678.300T^{-1}$
$\Delta Gf° = -422.245 - 23.144\times10^{-3}T\ln T + 2.209\times10^{-6}T^{2} + 339.150T^{-1} + 282.192\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Bennington (30). Low-temperature heat capacities and entropy at 298 K from Shomate (453). High-temperature data based on Naylor (351).

$Na_2Ti_3O_7$(c,l)
Sodium Trititanate
[Formation: $2Na(c,l,g) + 3Ti(c) + 3.5O_2(g) = Na_2Ti_3O_7(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	54.850	55.910	55.910	0	-832.100	-783.751	574.497
300	55.040	56.250	55.917	.100	-832.102	-783.448	570.734
371	60.457	68.667	57.172	4.265	-832.004	-771.933	454.727
371	60.457	68.667	57.172	4.265	-833.248	-771.933	454.727
400	62.670	73.300	58.175	6.050	-833.173	-767.143	419.142
500	66.730	87.760	62.700	12.530	-832.663	-750.700	328.127
600	69.300	100.170	67.920	19.350	-831.919	-734.365	267.489
700	71.020	110.990	73.319	26.370	-831.102	-718.155	224.215
800	72.240	120.560	78.647	33.530	-830.263	-702.092	191.800
900	73.170	129.130	83.786	40.810	-829.426	-686.114	166.609
1000	73.980	136.880	88.720	48.160	-828.625	-670.236	146.478
1100	74.810	143.970	93.425	55.600	-827.862	-654.455	130.027
1156	75.359	147.697	95.963	59.805	-827.443	-645.617	122.057
1156	75.359	147.697	95.963	59.805	-830.494	-645.617	122.057
1177	75.565	149.055	96.898	61.389	-830.273	-642.260	119.256
1177	75.565	149.055	96.898	61.389	-876.843	-642.260	119.256
1200	75.790	150.520	97.912	63.130	-876.507	-637.685	116.137
1300	77.050	156.630	102.192	70.770	-875.018	-617.832	103.866
1400	78.700	162.400	106.293	78.550	-873.479	-598.116	93.369
1401	78.720	162.450	106.327	78.630	-873.462	-597.911	93.270
1401	94.600	188.770	106.327	115.500	-836.592	-597.911	93.270
1500	94.600	195.230	111.983	124.870	-833.479	-581.152	84.673
1600	94.600	201.330	117.374	134.330	-830.428	-564.424	77.096
1700	94.600	207.070	122.488	143.790	-827.467	-547.895	70.436
1800	94.600	212.480	127.341	153.250	-824.617	-531.539	64.537

Phase changes:
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1401 K, melting point of $Na_2Ti_3O_7$; ΔH° = 36.870 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1401 K: $Cp° = 69.389 + 6.364\times10^{-3}T - 14.616\times10^{5}T^{-2}$
$H°- H°_{298} = 69.389\times10^{-3}T + 3.182\times10^{-6}T^{2} + 14.616\times10^{2}T^{-1} - 25.873$

1401-1800 K: $Cp° = 94.600$
$H°- H°_{298} = 94.600\times10^{-3}T - 17.035$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -841.210 + 19.751\times10^{-3}T - 11.264\times10^{-6}T^{2} + 1259.000T^{-1}$
$\Delta Gf° = -841.210 - 19.751\times10^{-3}T\ln T + 11.264\times10^{-6}T^{2} + 629.500T^{-1} + 294.813\times10^{-3}T$

371-1156 K: $\Delta Hf° = -841.986 + 13.645\times10^{-3}T - 1.764\times10^{-6}T^{2} + 1440.800T^{-1}$
$\Delta Gf° = -841.986 - 13.645\times10^{-3}T\ln T + 1.764\times10^{-6}T^{2} + 720.400T^{-1} + 263.645\times10^{-3}T$

1156-1177 K: $\Delta Hf° = -854.098 + 20.845\times10^{-3}T - 2.733\times10^{-6}T^{2} + 3789.500T^{-1}$
$\Delta Gf° = -854.098 - 20.845\times10^{-3}T\ln T + 2.733\times10^{-6}T^{2} + 1894.750T^{-1} + 322.902\times10^{-3}T$

1177-1401 K: $\Delta Hf° = -905.023 + 24.919\times10^{-3}T - 2.925\times10^{-6}T^{2} + 3585.700T^{-1}$
$\Delta Gf° = -905.023 - 24.919\times10^{-3}T\ln T + 2.925\times10^{-6}T^{2} + 1792.850T^{-1} + 394.823\times10^{-3}T$

1401-1800 K: $\Delta Hf° = -896.185 + 50.130\times10^{-3}T - 6.107\times10^{-6}T^{2} + 2124.100T^{-1}$
$\Delta Gf° = -896.185 - 50.130\times10^{-3}T\ln T + 6.107\times10^{-6}T^{2} + 1062.050T^{-1} + 567.081\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Bennington (30). Low-temperature heat capacities and entropy at 298 K from Shomate (453). High-temperature data based on Naylor (351).

$Na_2Ti_6O_{13}(c)$
Sodium Hexatitanate
[Formation: $2Na(c,l,g) + 6Ti(c) + 6.5O_2(g) = Na_2Ti_6O_{13}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	94.940	95.270	95.270	0	-1510.900	-1423.906	1043.738
300	95.210	95.858	95.271	.176	-1510.899	-1423.358	1036.903
371	103.361	117.059	97.451	7.274	-1510.676	-1402.659	826.272
371	103.361	117.059	97.451	7.274	-1511.920	-1402.659	826.272
400	106.690	124.963	99.163	10.320	-1511.754	-1394.124	761.704
500	113.708	149.585	106.849	21.368	-1510.797	-1364.825	596.557
600	118.103	170.736	115.778	32.975	-1509.524	-1335.748	486.540
700	120.888	189.167	124.974	44.935	-1508.167	-1306.858	408.014
800	122.751	205.438	134.036	57.122	-1506.835	-1278.206	349.185
900	124.197	219.981	142.790	69.472	-1505.583	-1249.693	303.463
1000	125.593	233.138	151.178	81.960	-1504.399	-1221.318	266.915
1100	127.183	245.181	159.184	94.597	-1503.306	-1193.103	237.045
1156	128.260	251.520	163.504	101.746	-1502.707	-1177.297	222.573
1156	128.260	251.520	163.504	101.746	-1508.809	-1177.297	222.573
1177	128.664	253.833	165.096	104.444	-1508.452	-1171.277	217.484
1177	128.664	253.833	165.096	104.444	-1555.022	-1171.277	217.484
1200	129.106	256.327	166.820	107.408	-1554.539	-1163.789	211.952
1300	131.388	266.749	174.111	120.430	-1552.398	-1131.308	190.188
1400	133.954	276.578	181.082	133.695	-1550.190	-1099.002	171.560
1500	136.623	285.911	187.762	147.224	-1547.870	-1066.853	155.438
1600	139.111	294.810	194.176	161.014	-1545.466	-1034.868	141.355

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp^\circ = 115.444 + 13.252\times10^{-3}T - 21.739\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 115.444\times10^{-3}T + 6.626\times10^{-6}T^{2} + 21.739\times10^{2}T^{-1} - 42.300$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -1524.034 + 27.685\times10^{-3}T - 12.698\times10^{-6}T^{2} + 1791.300T^{-1}$
$\Delta Gf^\circ = -1524.034 - 27.685\times10^{-3}T\ln T + 12.698\times10^{-6}T^{2} + 895.650T^{-1} + 479.705\times10^{-3}T$
371-1156 K: $\Delta Hf^\circ = -1524.810 + 21.579\times10^{-3}T - 3.198\times10^{-6}T^{2} + 1973.100T^{-1}$
$\Delta Gf^\circ = -1524.810 - 21.579\times10^{-3}T\ln T + 3.198\times10^{-6}T^{2} + 986.550T^{-1} + 448.538\times10^{-3}T$
1156-1177 K: $\Delta Hf^\circ = -1549.032 + 35.979\times10^{-3}T - 5.135\times10^{-6}T^{2} + 6670.500T^{-1}$
$\Delta Gf^\circ = -1549.032 - 35.979\times10^{-3}T\ln T + 5.135\times10^{-6}T^{2} + 3335.250T^{-1} + 567.053\times10^{-3}T$
1177-1600 K: $\Delta Hf^\circ = -1599.958 + 40.053\times10^{-3}T - 5.327\times10^{-6}T^{2} + 6466.700T^{-1}$
$\Delta Gf^\circ = -1599.958 - 40.053\times10^{-3}T\ln T + 5.327\times10^{-6}T^{2} + 3233.350T^{-1} + 638.974\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Bennington (30). Low-temperature heat capacities and entropy at 298 K from Stuve (480). High-temperature data from Ferrante (146).

$NaUO_3(c)$
Sodium Uranium Trioxide
[Formation: $Na(c,l) + U(c) + 1.5O_2(g) = NaUO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	26.020	31.750	31.750	0	-357.220	-337.526	247.410
300	26.066	31.911	31.751	.048	-357.215	-337.402	245.794
371	27.320	37.604	32.339	1.953	-357.049	-332.732	196.004
371	27.320	37.604	32.339	1.953	-357.671	-332.732	196.004
400	27.832	39.679	32.797	2.753	-357.605	-330.785	180.730
500	28.882	46.010	34.826	5.592	-357.340	-324.109	141.666
600	29.649	51.347	37.147	8.520	-357.063	-317.489	115.644
700	30.283	55.966	39.513	11.517	-356.807	-310.915	97.071
800	30.845	60.047	41.830	14.574	-356.594	-304.375	83.150
900	31.367	63.710	44.060	17.685	-356.444	-297.856	72.328
942	31.575	65.145	44.968	19.007	-356.403	-295.123	68.470
942	31.575	65.145	44.968	19.007	-357.070	-295.123	68.470
1000	31.863	67.041	46.195	20.846	-356.948	-291.314	63.666

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 27.831 + 4.302\times10^{-3}T - 2.750\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 27.831\times10^{-3}T + 2.151\times10^{-6}T^{2} + 2.750\times10^{2}T^{-1} - 9.411$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -360.502 + 9.925\times10^{-3}T - 7.484\times10^{-6}T^{2} + 294.700T^{-1}$
$\Delta Gf^\circ = -360.502 - 9.925\times10^{-3}T\ln T + 7.484\times10^{-6}T^{2} + 147.350T^{-1} + 129.724\times10^{-3}T$
371-942 K: $\Delta Hf^\circ = -360.891 + 6.872\times10^{-3}T - 2.734\times10^{-6}T^{2} + 385.600T^{-1}$
$\Delta Gf^\circ = -360.891 - 6.872\times10^{-3}T\ln T + 2.734\times10^{-6}T^{2} + 192.800T^{-1} + 114.140\times10^{-3}T$
942-1000 K: $\Delta Hf^\circ = -358.480 - 0.273\times10^{-3}T + 1.489\times10^{-6}T^{2} + 298.100T^{-1}$
$\Delta Gf^\circ = -358.480 + 0.273\times10^{-3}T\ln T - 1.489\times10^{-6}T^{2} + 149.050T^{-1} + 66.679\times10^{-3}T$

Source: Data from Cordfunke (98).

$Na_2UO_4(\alpha)$
α-Disodium Uranium Tetroxide
[Formation: $2Na(c,l,g) + U(c,l) + 2O_2(g) = Na_2UO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	35.050	39.680	39.680	0	-453.470	-425.168	311.652
300	35.140	39.900	39.683	.065	-453.467	-424.991	309.602
371	37.306	47.629	40.475	2.654	-453.370	-418.261	246.387
371	37.306	47.629	40.475	2.654	-454.614	-418.261	246.387
400	38.190	50.470	41.097	3.749	-454.577	-415.421	226.972
500	39.940	59.200	43.878	7.661	-454.345	-405.658	177.311
600	41.170	66.590	47.058	11.719	-454.036	-395.946	144.221
700	42.160	73.020	50.324	15.887	-453.704	-386.296	120.606
800	43.010	78.700	53.517	20.146	-453.384	-376.686	102.904
900	43.800	83.810	56.602	24.487	-453.100	-367.112	89.146
942	44.107	85.815	57.860	26.333	-452.998	-363.102	84.241
942	44.107	85.815	57.860	26.333	-453.665	-363.102	84.241
1000	44.530	88.470	59.566	28.904	-453.452	-357.540	78.139
1049	44.878	90.609	60.966	31.094	-453.263	-352.844	73.511
1049	44.878	90.609	60.966	31.094	-454.400	-352.844	73.511
1100	45.240	92.740	62.383	33.393	-454.139	-347.907	69.122
1177	45.770	95.821	64.473	36.897	-453.724	-340.479	63.221
1177	45.770	95.821	64.473	36.897	-500.294	-340.479	63.221
1193	45.880	96.440	64.898	37.630	-500.142	-338.312	61.976

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1193 K: $Cp° = 38.848 + 6.186\times10^{-3}T - 5.011\times10^{5}T^{-2}$
$H°- H°_{298} = 38.848\times10^{-3}T + 3.093\times10^{-6}T^{2} + 5.011\times10^{2}T^{-1} - 13.538$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -458.111 + 13.376\times10^{-3}T - 11.451\times10^{-6}T^{2} + 498.200T^{-1}$
$\Delta Gf° = -458.111 - 13.376\times10^{-3}T\ln T + 11.451\times10^{-6}T^{2} + 249.100T^{-1} + 180.487\times10^{-3}T$
371-942 K: $\Delta Hf° = -458.887 + 7.270\times10^{-3}T - 1.951\times10^{-6}T^{2} + 680.000T^{-1}$
$\Delta Gf° = -458.887 - 7.270\times10^{-3}T\ln T + 1.951\times10^{-6}T^{2} + 340.000T^{-1} + 149.319\times10^{-3}T$
942-1049 K: $\Delta Hf° = -456.477 + 0.125\times10^{-3}T + 2.271\times10^{-6}T^{2} + 592.500T^{-1}$
$\Delta Gf° = -456.477 - 0.125\times10^{-3}T\ln T - 2.271\times10^{-6}T^{2} + 296.250T^{-1} + 101.858\times10^{-3}T$
1049-1177 K: $\Delta Hf° = -458.773 + 1.230\times10^{-3}T + 2.271\times10^{-6}T^{2} + 592.500T^{-1}$
$\Delta Gf° = -458.773 - 1.230\times10^{-3}T\ln T - 2.271\times10^{-6}T^{2} + 296.250T^{-1} + 111.733\times10^{-3}T$
1177-1193 K: $\Delta Hf° = -509.699 + 5.304\times10^{-3}T + 2.079\times10^{-6}T^{2} + 388.700T^{-1}$
$\Delta Gf° = -509.699 - 5.304\times10^{-3}T\ln T - 2.079\times10^{-6}T^{2} + 194.350T^{-1} + 183.654\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cordfunke (98). Other data from Fredrickson (160).

$Na_2U_2O_7$(c)
Disodium Diuranium Heptaoxide
[Formation: $2Na(c,l) + 2U(c) + 3.5O_2(g) = Na_2U_2O_7(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	54.316	65.932	65.932	0	-763.550	-717.581	525.994
300	54.441	66.269	65.932	.101	-763.542	-717.293	522.541
371	57.621	78.243	67.170	4.108	-763.263	-706.379	416.111
371	57.621	78.243	67.170	4.108	-764.507	-706.379	416.111
400	58.920	82.629	68.134	5.798	-764.391	-701.840	383.463
500	61.174	96.042	72.414	11.814	-763.887	-686.255	299.958
600	62.555	107.326	77.318	18.005	-763.375	-670.778	244.328
700	63.523	117.046	82.316	24.311	-762.940	-655.382	204.617
800	64.271	125.578	87.201	30.702	-762.637	-640.042	174.849
900	64.890	133.186	91.896	37.161	-762.505	-624.726	151.702
942	65.117	136.151	93.804	39.891	-762.512	-618.297	143.447
942	65.117	136.151	93.804	39.891	-763.846	-618.297	143.447
1000	65.430	140.050	96.373	43.677	-763.734	-609.339	133.169

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K:
$$Cp^\circ = 62.889 + 3.390\text{x}10^{-3}T - 8.519\text{x}10^{5}T^{-2}$$
$$H^\circ - H^\circ_{298} = 62.889\text{x}10^{-3}T + 1.695\text{x}10^{-6}T^2 + 8.519\text{x}10^{2}T^{-1} - 21.758$$

Formation equations (kcal/mol):

298.15-371 K:
$$\Delta Hf^\circ = -771.874 + 23.462\text{x}10^{-3}T - 17.825\text{x}10^{-6}T^2 + 868.700T^{-1}$$
$$\Delta Gf^\circ = -771.874 - 23.462\text{x}10^{-3}T\ln T + 17.825\text{x}10^{-6}T^2 + 434.350T^{-1} + 305.577\text{x}10^{-3}T$$

371-942 K:
$$\Delta Hf^\circ = -772.651 + 17.356\text{x}10^{-3}T - 8.325\text{x}10^{-6}T^2 + 1050.500T^{-1}$$
$$\Delta Gf^\circ = -772.651 - 17.356\text{x}10^{-3}T\ln T + 8.325\text{x}10^{-6}T^2 + 525.250T^{-1} + 274.410\text{x}10^{-3}T$$

942-1000 K:
$$\Delta Hf^\circ = -767.830 + 3.066\text{x}10^{-3}T + 0.118\text{x}10^{-6}T^2 + 875.500T^{-1}$$
$$\Delta Gf^\circ = -767.830 - 3.066\text{x}10^{-3}T\ln T - 0.118\text{x}10^{-6}T^2 + 437.750T^{-1} + 179.488\text{x}10^{-3}T$$

Source: Data from Cordfunke (98).

$Na_3UO_4(c)$
Trisodium Uranium Tetroxide
[Formation: $3Na(c,l,g) + U(c) + 2O_2(g) = Na_3UO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	41.350	47.370	47.370	0	-477.700	-448.024	328.406
300	41.430	47.630	47.373	.077	-477.697	-447.838	326.246
371	43.574	56.698	48.310	3.112	-477.658	-440.778	259.652
371	43.574	56.698	48.310	3.112	-479.524	-440.778	259.652
400	44.450	60.010	49.040	4.388	-479.524	-437.749	239.172
500	46.170	70.130	52.280	8.925	-479.408	-427.316	186.777
600	47.380	78.650	55.975	13.605	-479.198	-416.910	151.857
700	48.350	86.030	59.754	18.393	-478.952	-406.551	126.929
800	49.190	92.540	63.453	23.270	-478.709	-396.225	108.242
900	49.950	98.380	67.017	28.227	-478.499	-385.928	93.715
942	50.252	100.665	68.466	30.331	-478.429	-381.610	88.535
942	50.252	100.665	68.466	30.331	-479.096	-381.610	88.535
1000	50.670	103.680	70.421	33.259	-478.926	-375.612	82.089
1049	51.008	106.112	72.032	35.750	-478.776	-370.552	77.200
1049	51.008	106.112	72.032	35.750	-479.913	-370.552	77.200
1100	51.360	108.540	73.667	38.360	-479.697	-365.243	72.566
1177	51.876	112.035	76.067	42.334	-479.352	-357.234	66.332
1177	51.876	112.035	76.067	42.334	-549.207	-357.234	66.332
1200	52.030	113.040	76.766	43.529	-548.962	-353.492	64.379

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 45.148 + 6.018\times10^{-3}T - 4.972\times10^{5}T^{-2}$

$H°-H°_{298} = 45.148\times10^{-3}T + 3.009\times10^{-6}T^{2} + 4.972\times10^{2}T^{-1} - 15.396$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -482.607 + 15.725\times10^{-3}T - 16.193\times10^{-6}T^{2} + 494.300T^{-1}$

$\Delta Gf° = -482.607 - 15.725\times10^{-3}T\ln T + 16.193\times10^{-6}T^{2} + 247.150T^{-1} + 197.978\times10^{-3}T$

371-942 K: $\Delta Hf° = -483.771 + 6.566\times10^{-3}T - 1.943\times10^{-6}T^{2} + 767.000T^{-1}$

$\Delta Gf° = -483.771 - 6.566\times10^{-3}T\ln T + 1.943\times10^{-6}T^{2} + 383.500T^{-1} + 151.227\times10^{-3}T$

942-1049 K: $\Delta Hf° = -481.361 - 0.579\times10^{-3}T + 2.279\times10^{-6}T^{2} + 679.500T^{-1}$

$\Delta Gf° = -481.361 + 0.579\times10^{-3}T\ln T - 2.279\times10^{-6}T^{2} + 339.750T^{-1} + 103.765\times10^{-3}T$

1049-1177 K: $\Delta Hf° = -483.657 + 0.526\times10^{-3}T + 2.279\times10^{-6}T^{2} + 679.500T^{-1}$

$\Delta Gf° = -483.657 - 0.526\times10^{-3}T\ln T - 2.279\times10^{-6}T^{2} + 339.750T^{-1} + 113.640\times10^{-3}T$

1177-1200 K: $\Delta Hf° = -560.046 + 6.637\times10^{-3}T + 1.991\times10^{-6}T^{2} + 373.800T^{-1}$

$\Delta Gf° = -560.046 - 6.637\times10^{-3}T\ln T - 1.991\times10^{-6}T^{2} + 186.900T^{-1} + 221.522\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from O'Hare (372). Other data from Fredrickson (157).

$Na_2WO_4(c,l)$
Sodium Tungstate
[Formation: $2Na(c,l,g) + W(c) + 2O_2(g) = Na_2WO_4(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	33.400	38.540	38.540	0	-370.200	-342.810	251.283
300	33.491	38.747	38.540	.062	-370.199	-342.638	249.608
371	36.179	46.224	39.310	2.565	-370.124	-336.122	198.001
371	36.179	46.224	39.310	2.565	-371.368	-336.122	198.001
400	37.277	48.988	39.913	3.630	-371.330	-333.368	182.142
500	39.473	57.556	42.608	7.474	-371.036	-323.907	141.578
600	41.131	64.905	45.727	11.507	-370.573	-314.526	114.565
700	42.535	71.353	48.936	15.692	-369.982	-305.229	95.295
800	43.804	77.117	52.104	20.010	-369.282	-296.028	80.870
860	44.525	80.311	53.962	22.660	-368.818	-290.546	73.835
860	45.506	89.078	53.962	30.200	-361.278	-290.546	73.835
900	47.888	91.201	55.570	32.068	-360.873	-287.265	69.757
967	51.876	94.781	58.162	35.410	-359.991	-281.815	63.692
967	51.670	101.668	58.162	42.070	-353.331	-281.815	63.692
1000	51.670	103.402	59.627	43.775	-352.845	-279.383	61.058
1100	51.670	108.327	63.834	48.942	-351.401	-272.101	54.061
1177	51.670	111.822	66.860	52.921	-350.316	-266.585	49.500
1177	51.670	111.822	66.860	52.921	-396.886	-266.585	49.500
1200	51.670	112.822	67.731	54.109	-396.474	-264.047	48.089

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
860 K, α - β transition point of Na_2WO_4; ΔH° = 7.540 kcal/mol.
967 K, melting point of Na_2WO_4; ΔH° = 6.660 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-860 K: $Cp° = 36.476 + 10.184\text{x}10^{-3}T - 5.236\text{x}10^{5}T^{-2}$
$H°- H°_{298} = 36.476\text{x}10^{-3}T + 5.092\text{x}10^{-6}T^{2} + 5.236\text{x}10^{2}T^{-1} - 13.084$
860-967 K: $Cp° = -5.691 + 59.530\text{x}10^{-3}T$
$H°- H°_{298} = -5.691\text{x}10^{-3}T + 29.765\text{x}10^{-6}T^{2} + 13.080$
967-1200 K: $Cp° = 51.670$
$H°- H°_{298} = 51.670\text{x}10^{-3}T - 7.895$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -373.559 + 8.299\text{x}10^{-3}T - 5.601\text{x}10^{-6}T^{2} + 412.200T^{-1}$
$\Delta Gf° = -373.559 - 8.299\text{x}10^{-3}T\ln T + 5.601\text{x}10^{-6}T^{2} + 206.100T^{-1} + 146.428\text{x}10^{-3}T$
371-860 K: $\Delta Hf° = -374.335 + 2.193\text{x}10^{-3}T + 3.899\text{x}10^{-6}T^{2} + 594.000T^{-1}$
$\Delta Gf° = -374.335 - 2.193\text{x}10^{-3}T\ln T - 3.899\text{x}10^{-6}T^{2} + 297.000T^{-1} + 115.260\text{x}10^{-3}T$
860-967 K: $\Delta Hf° = -348.171 - 39.974\text{x}10^{-3}T + 28.572\text{x}10^{-6}T^{2} + 70.400T^{-1}$
$\Delta Gf° = -348.171 + 39.974\text{x}10^{-3}T\ln T - 28.572\text{x}10^{-6}T^{2} + 35.200T^{-1} - 178.510\text{x}10^{-3}T$
967-1177 K: $\Delta Hf° = -369.146 + 17.387\text{x}10^{-3}T - 1.193\text{x}10^{-6}T^{2} + 70.400T^{-1}$
$\Delta Gf° = -369.146 - 17.387\text{x}10^{-3}T\ln T + 1.193\text{x}10^{-6}T^{2} + 35.200T^{-1} + 208.709\text{x}10^{-3}T$
1177-1200 K: $\Delta Hf° = -420.072 + 21.461\text{x}10^{-3}T - 1.385\text{x}10^{-6}T^{2} - 133.400T^{-1}$
$\Delta Gf° = -420.072 - 21.461\text{x}10^{-3}T\ln T + 1.385\text{x}10^{-6}T^{2} - 66.700T^{-1} + 280.630\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from King (271). High-temperature data based on Denielou (117).

$Na_2ZrO_3(c)$
Sodium Zirconate
[Formation: $2Na(c,l) + Zr(c) + 1.5O_2(g) = Na_2ZrO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	30.086	29.995	29.995	0	-403.000	-379.915	278.481
300	30.164	30.181	29.995	.056	-402.999	-379.769	276.658
371	32.995	36.925	30.687	2.314	-402.951	-374.277	220.477
371	32.995	36.925	30.687	2.314	-404.195	-374.277	220.477
400	34.151	39.452	31.232	3.288	-404.160	-371.940	203.216
500	36.525	47.351	33.687	6.832	-403.861	-363.913	159.064
600	37.873	54.142	36.544	10.559	-403.401	-355.965	129.658
700	38.610	60.041	39.488	14.387	-402.865	-348.102	108.681
800	39.007	65.225	42.388	18.270	-402.303	-340.318	92.969
900	39.232	69.834	45.186	22.183	-401.745	-332.602	80.766
1000	39.368	73.975	47.862	26.113	-401.211	-324.949	71.017
1025*	39.393	74.947	48.510	27.098	-401.082	-323.043	68.878
1100	41.826	77.943	50.414	30.282	-400.486	-317.354	63.052
1110	39.420	78.302	50.663	30.679	-400.437	-316.598	62.335
1125	39.413	78.831	51.035	31.270	-400.368	-315.466	61.284
1136	39.404	79.214	51.306	31.703	-400.318	-314.636	60.531
1136	39.404	79.214	51.306	31.703	-401.269	-314.636	60.531
1150	39.393	79.697	51.649	32.255	-401.182	-313.561	59.589
1170	39.372	80.376	52.134	33.043	-401.065	-312.037	58.286

*A nonisothermal transition occurs between 1025 and 1110 K. The equations below assume a second order transition at 1100 K.

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 37.164 + 4.076\times10^{-3}T - 7.371\times10^{5}T^{-2}$
$H°-H°_{298} = 37.164\times10^{-3}T + 2.038\times10^{-6}T^2 + 7.371\times10^{2}T^{-1} - 13.734$
1100-1170 K: $Cp° = 43.327 - 3.422\times10^{-3}T$
$H°-H°_{298} = 43.327\times10^{-3}T - 1.711\times10^{-6}T^2 - 15.307$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -408.041 + 12.424\times10^{-3}T - 8.975\times10^{-6}T^2 + 636.400T^{-1}$
$\Delta Gf° = -408.041 - 12.424\times10^{-3}T\ln T + 8.975\times10^{-6}T^2 + 318.200T^{-1} + 158.868\times10^{-3}T$
371-1100 K: $\Delta Hf° = -408.817 + 6.318\times10^{-3}T + 0.525\times10^{-6}T^2 + 818.200T^{-1}$
$\Delta Gf° = -408.817 - 6.318\times10^{-3}T\ln T - 0.525\times10^{-6}T^2 + 409.100T^{-1} + 127.700\times10^{-3}T$
1100-1136 K: $\Delta Hf° = -410.390 + 12.481\times10^{-3}T - 3.224\times10^{-6}T^2 + 81.100T^{-1}$
$\Delta Gf° = -410.390 - 12.481\times10^{-3}T\ln T + 3.224\times10^{-6}T^2 + 40.550T^{-1} + 168.470\times10^{-3}T$
1136-1170 K: $\Delta Hf° = -412.886 + 13.650\times10^{-3}T - 3.092\times10^{-6}T^2 + 135.600T^{-1}$
$\Delta Gf° = -412.886 - 13.650\times10^{-3}T\ln T + 3.092\times10^{-6}T^2 + 67.800T^{-1} + 179.019\times10^{-3}T$

Source: Data from Beyer (39).

$NbB_{1.97}(c)$
Niobium Boride
[Formation: $Nb(c) + 1.97B(\beta) = NbB_{1.97}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^{\circ}_{298})/T$	$H°- H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15*	11.410	8.910	8.910	0	-60.000	-59.234	43.419
300	11.490	8.980	8.913	.020	-60.001	-59.228	43.147
400	14.350	12.730	9.405	1.330	-59.915	-58.987	32.229
500	15.800	16.110	10.410	2.850	-59.812	-58.761	25.684
600	16.690	19.070	11.620	4.470	-59.751	-58.565	21.332
700	17.320	21.690	12.861	6.180	-59.694	-58.362	18.221
800	17.800	24.040	14.128	7.930	-59.664	-58.183	15.895
900	18.210	26.160	15.349	9.730	-59.637	-57.998	14.084
1000	18.560	28.100	16.530	11.570	-59.619	-57.817	12.636
1100	18.890	29.880	17.653	13.450	-59.603	-57.639	11.452
1200	19.190	31.540	18.748	15.350	-59.606	-57.447	10.462
1300	19.470	33.080	19.788	17.280	-59.619	-57.248	9.624
1400	19.740	34.540	20.797	19.240	-59.642	-57.081	8.911
1500	20.010	35.910	21.757	21.230	-59.681	-56.883	8.288
1600	20.270	37.210	22.685	23.240	-59.746	-56.718	7.747
1700	20.520	38.440	23.569	25.280	-59.824	-56.509	7.265
1800	20.770	39.620	24.426	27.350	-59.917	-56.285	6.834
1900	21.010	40.750	25.255	29.440	-60.035	-56.091	6.452
2000	21.260	41.840	26.065	31.550	-60.181	-55.911	6.110
2100	21.500	42.880	26.837	33.690	-60.345	-55.675	5.794

*Enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2100 K: $Cp° = 16.821 + 2.284x10^{-3}T - 5.412x10^{5}T^{-2}$
$H°- H^{\circ}_{298} = 16.821x10^{-3}T + 1.142x10^{-6}T^{2} + 5.412x10^{2}T^{-1} - 6.932$

Formation equations (kcal/mol):

298.15-2100 K: $\Delta Hf° = -61.024 + 2.321x10^{-3}T - 0.993x10^{-6}T^{2} + 125.445T^{-1}$
$\Delta Gf° = -61.024 - 2.321x10^{-3}TlnT + 0.993x10^{-6}T^{2} + 62.723T^{-1} + 18.224x10^{-3}T$

Sources: Enthalpy of formation at 298 K estimated using Johnson (219). Low-temperature capacities and entropy at 298 K from Westrum (525). High-temperature data based on Mezaki (331) and Bolgar (49).

$NbC_{0.5}(c)$
Niobium Carbide
[Formation: $Nb(c) + 0.5C(c) = NbC_{0.5}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.234	7.650	7.650	0	-22.700	-22.182	16.260
300	7.251	7.695	7.652	.013	-22.700	-22.179	16.157
400	7.900	9.880	7.943	.775	-22.660	-22.011	12.026
500	8.280	11.687	8.517	1.585	-22.624	-21.855	9.553
600	8.556	13.222	9.177	2.427	-22.593	-21.702	7.905
700	8.781	14.558	9.852	3.294	-22.571	-21.560	6.731
800	8.980	15.743	10.516	4.182	-22.557	-21.415	5.850
900	9.164	16.812	11.156	5.090	-22.544	-21.272	5.165
1000	9.338	17.786	11.771	6.015	-22.537	-21.130	4.618
1100	9.506	18.684	12.359	6.957	-22.531	-20.987	4.170
1200	9.669	19.518	12.921	7.916	-22.524	-20.833	3.794
1300	9.830	20.299	13.460	8.891	-22.518	-20.688	3.478
1400	9.988	21.033	13.975	9.881	-22.514	-20.553	3.208
1500	10.145	21.727	14.468	10.888	-22.514	-20.410	2.974
1600	10.300	22.387	14.943	11.910	-22.518	-20.265	2.768
1700	10.455	23.016	15.400	12.948	-22.526	-20.120	2.587
1800	10.609	23.618	15.840	14.001	-22.539	-19.981	2.426
1900	10.762	24.196	16.264	15.070	-22.556	-19.852	2.283
2000	10.915	24.752	16.675	16.154	-22.581	-19.700	2.153

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.940 + 1.500\text{x}10^{-3}T - 1.025\text{x}10^{5}T^{-2}$

$H°-H°_{298} = 7.940\text{x}10^{-3}T + 0.750\text{x}10^{-6}T^{2} + 1.025\text{x}10^{2}T^{-1} - 2.778$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -23.082 + 0.985\text{x}10^{-3}T - 0.405\text{x}10^{-6}T^{2} + 36.950T^{-1}$

$\Delta Gf° = -23.082 - 0.985\text{x}10^{-3}T\ln T + 0.405\text{x}10^{-6}T^{2} + 18.475T^{-1} + 8.299\text{x}10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (515). Other data from Schick (437).

$NbC_{0.75}(c)$
Niobium Carbide
[Formation: $Nb(c) + 0.75C(c) = NbC_{0.75}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.100	7.720	7.720	0	-29.300	-28.701	21.038
300	8.123	7.770	7.720	.015	-29.299	-28.696	20.905
400	9.018	10.240	8.047	.877	-29.220	-28.507	15.575
500	9.558	12.320	8.706	1.807	-29.143	-28.343	12.388
600	9.958	14.100	9.460	2.784	-29.071	-28.186	10.267
700	10.290	15.660	10.236	3.797	-29.010	-28.047	8.757
800	10.590	17.050	10.999	4.841	-28.954	-27.910	7.625
900	10.860	18.310	11.740	5.913	-28.899	-27.780	6.746
1000	11.120	19.470	12.458	7.012	-28.844	-27.660	6.045
1100	11.360	20.540	13.144	8.136	-28.787	-27.538	5.471
1200	11.600	21.540	13.803	9.284	-28.726	-27.418	4.993
1300	11.840	22.480	14.434	10.460	-28.656	-27.305	4.590
1400	12.070	23.370	15.049	11.650	-28.593	-27.220	4.249
1500	12.290	24.210	15.630	12.870	-28.522	-27.120	3.951
1600	12.510	25.010	16.191	14.110	-28.451	-27.023	3.691
1700	12.720	25.770	16.729	15.370	-28.382	-26.926	3.462
1800	12.940	26.500	17.250	16.650	-28.315	-26.841	3.259
1900	13.150	27.210	17.757	17.960	-28.239	-26.779	3.080
2000	13.350	27.890	18.250	19.280	-28.177	-26.700	2.918

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 9.025 + 2.216\times10^{-3}T - 1.410\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 9.025\times10^{-3}T + 1.108\times10^{-6}T^{2} + 1.410\times10^{2}T^{-1} - 3.262$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -29.742 + 1.191\times10^{-3}T - 0.238\times10^{-6}T^{2} + 32.375T^{-1}$

$\Delta Gf^\circ = -29.742 - 1.191\times10^{-3}T\ln T + 0.238\times10^{-6}T^{2} + 16.187T^{-1} + 10.022\times10^{-3}T$

Source: Data from Storms (474).

$NbC_{0.87}(c)$
Niobium Carbide
[Formation: $Nb(c) + 0.87C(c) = NbC_{0.87}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	8.510	7.980	7.980	0	-31.900	-31.329	22.965
300	8.537	8.033	7.980	.016	-31.898	-31.325	22.820
400	9.536	10.640	8.328	.925	-31.802	-31.149	17.019
500	10.100	12.840	9.022	1.909	-31.709	-31.001	13.550
600	10.500	14.710	9.810	2.940	-31.629	-30.859	11.240
700	10.810	16.360	10.637	4.006	-31.564	-30.746	9.599
800	11.080	17.820	11.444	5.101	-31.513	-30.630	8.368
900	11.330	19.140	12.227	6.222	-31.467	-30.522	7.412
1000	11.570	20.340	12.974	7.366	-31.429	-30.413	6.647
1100	11.790	21.460	13.702	8.534	-31.390	-30.315	6.023
1200	12.010	22.490	14.387	9.724	-31.351	-30.203	5.501
1300	12.220	23.460	15.045	10.940	-31.308	-30.099	5.060
1400	12.440	24.380	15.687	12.170	-31.271	-30.025	4.687
1500	12.650	25.240	16.293	13.420	-31.238	-29.931	4.361
1600	12.860	26.060	16.872	14.700	-31.197	-29.830	4.075
1700	13.060	26.850	17.444	15.990	-31.168	-29.757	3.825
1800	13.270	27.600	17.983	17.310	-31.131	-29.668	3.602
1900	13.480	28.320	18.504	18.650	-31.096	-29.593	3.404
2000	13.690	29.020	19.015	20.010	-31.066	-29.510	3.225

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.764 + 1.972\times10^{-3}T - 1.638\times10^{5}T^{-2}$

$H°-H°_{298} = 9.764\times10^{-3}T + 0.986\times10^{-6}T^{2} + 1.638\times10^{2}T^{-1} - 3.548$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -32.425 + 1.507\times10^{-3}T - 0.452\times10^{-6}T^{2} + 34.499T^{-1}$

$\Delta Gf° = -32.425 - 1.507\times10^{-3}T\ln T + 0.452\times10^{-6}T^{2} + 17.250T^{-1} + 11.933\times10^{-3}T$

Source: Data from Storms (474).

$NbC_{0.98}(c)$
Niobium Carbide
[Formation: $Nb(c) + 0.98C(c) = NbC_{0.98}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.660	8.357	8.357	0	-33.200	-32.697	23.967
300	8.695	8.411	8.358	.016	-33.199	-32.693	23.817
400	10.010	11.105	8.715	.956	-33.098	-32.540	17.779
500	10.790	13.427	9.431	1.998	-32.982	-32.415	14.168
600	11.320	15.444	10.269	3.105	-32.867	-32.309	11.768
700	11.690	17.217	11.137	4.256	-32.765	-32.228	10.062
800	11.980	18.798	11.998	5.440	-32.674	-32.158	8.785
900	12.210	20.223	12.834	6.650	-32.594	-32.097	7.794
1000	12.410	21.520	13.639	7.881	-32.524	-32.046	7.003
1100	12.580	22.711	14.411	9.130	-32.462	-31.994	6.356
1200	12.740	23.812	15.148	10.397	-32.405	-31.944	5.818
1300	12.890	24.838	15.855	11.678	-32.357	-31.902	5.363
1400	13.027	25.798	16.531	12.974	-32.316	-31.874	4.976
1500	13.160	26.701	17.179	14.283	-32.287	-31.842	4.639
1600	13.290	27.555	17.801	15.606	-32.265	-31.807	4.345
1700	13.416	28.364	18.399	16.941	-32.256	-31.776	4.085
1800	13.540	29.135	18.974	18.289	-32.255	-31.750	3.855
1900	13.660	29.870	19.528	19.649	-32.265	-31.735	3.650
2000	13.780	30.574	20.063	21.021	-32.289	-31.697	3.464
2100	13.900	31.249	20.580	22.405	-32.325	-31.678	3.297
2200	14.020	31.898	21.079	23.801	-32.375	-31.637	3.143
2300	14.140	32.524	21.564	25.209	-32.438	-31.596	3.002
2400	14.260	33.129	22.034	26.629	-32.518	-31.565	2.874
2500	14.380	33.713	22.489	28.061	-32.611	-31.511	2.755

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 11.299 + 1.298\times10^{-3}T - 2.690\times10^{5}T^{-2}$

$H°- H°_{298} = 11.299\times10^{-3}T + 0.649\times10^{-6}T^{2} + 2.690\times10^{2}T^{-1} - 4.329$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -34.319 + 2.655\times10^{-3}T - 0.874\times10^{-6}T^{2} + 120.746T^{-1}$

$\Delta Gf° = -34.319 - 2.655\times10^{-3}T\ln T + 0.874\times10^{-6}T^{2} + 60.373T^{-1} + 19.630\times10^{-3}T$

2000-2500 K: $\Delta Hf° = -32.367 + 0.575\times10^{-3}T - 0.254\times10^{-6}T^{2} - 416.000T^{-1}$

$\Delta Gf° = -32.367 - 0.575\times10^{-3}T\ln T + 0.254\times10^{-6}T^{2} - 208.000T^{-1} + 4.146\times10^{-3}T$

Source: Data from Chase (83).

NbN(c)
Niobium Nitride
[Formation: Nb(c) + 0.5N_2(g) = NbN(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	9.320	8.250	8.250	0	-56.200	-49.243	36.095
300*	9.350	8.308	8.258	.015	-56.203	-49.201	35.842
400	10.710	11.201	8.639	1.025	-56.141	-46.874	25.610
500	11.580	13.691	9.401	2.145	-55.987	-44.571	19.482
600	12.210	15.861	10.303	3.335	-55.777	-42.306	15.410
700	12.710	17.782	11.239	4.580	-55.529	-40.086	12.515
800	13.110	19.506	12.162	5.875	-55.249	-37.895	10.352
900	13.450	21.070	13.070	7.200	-54.956	-35.744	8.680
1000	13.740	22.502	13.942	8.560	-54.647	-33.625	7.349
1100	13.990	23.823	14.782	9.945	-54.330	-31.542	6.267
1200	14.220	25.051	15.584	11.360	-53.998	-29.462	5.366
1300	14.420	26.197	16.359	12.790	-53.667	-27.426	4.611
1400	14.600	27.273	17.102	14.240	-53.335	-25.428	3.969
1500	14.770	28.286	17.813	15.710	-53.003	-23.443	3.416
1600	14.920	29.244	18.497	17.195	-52.675	-21.478	2.934
1643	14.970	29.640	18.785	17.835	-52.538	-20.643	2.746
1643	15.000	30.249	18.785	18.835	-51.538	-20.643	2.746
1700	15.000	30.760	19.178	19.690	-51.356	-19.570	2.516
1800	15.000	31.618	19.846	21.190	-51.052	-17.712	2.151
1900	15.000	32.429	20.487	22.690	-50.769	-15.882	1.827
2000	15.000	33.198	21.103	24.190	-50.508	-14.043	1.534

*Data above 298 K estimated.

Phase change: 1643 K, α - β transition point of NbN; ΔH° = 1.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1643 K: $Cp^\circ = 11.637 + 2.232\times10^{-3}T - 2.653\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 11.637\times10^{-3}T + 1.116\times10^{-6}T^2 + 2.653\times10^{2}T^{-1} - 4.459$

1643-2000 K: $Cp^\circ = 15.000$

$H^\circ - H^\circ_{298} = 15.000\times10^{-3}T - 5.810$

Formation equations (kcal/mol):

298.15-1643 K: $\Delta Hf^\circ = -58.125 + 3.183\times10^{-3}T + 0.049\times10^{-6}T^2 + 289.850T^{-1}$

$\Delta Gf^\circ = -58.125 - 3.183\times10^{-3}T\ln T - 0.049\times10^{-6}T^2 + 144.925T^{-1} + 46.310\times10^{-3}T$

1643-2000 K: $\Delta Hf^\circ = -59.477 + 6.545\times10^{-3}T - 1.067\times10^{-6}T^2 + 24.550T^{-1}$

$\Delta Gf^\circ = -59.477 - 6.545\times10^{-3}T\ln T + 1.067\times10^{-6}T^2 + 12.275T^{-1} + 70.249\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Low-temperature heat capacities and entropy at 298 K from Paukov (395). High-temperature data estimated following Kelley (243) and Schick (437).

$Nb_2N(c)$
Diniobium Nitride
[Formation: $2Nb(c) + 0.5N_2(g) = Nb_2N(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.130	19.000	19.000	0	-59.900	-53.554	39.256
300	16.138	19.100	19.000	.030	-59.899	-53.513	38.983
400	16.547	23.798	19.638	1.664	-59.813	-51.401	28.084
500	16.956	27.535	20.855	3.340	-59.719	-49.310	21.553
600	17.364	30.662	22.235	5.056	-59.605	-47.233	17.204
700	17.773	33.369	23.638	6.812	-59.479	-45.189	14.108
800	18.182	35.769	25.007	8.610	-59.340	-43.156	11.790
900	18.591	37.935	26.325	10.449	-59.185	-41.139	9.990
1000	19.000	39.914	27.586	12.328	-59.021	-39.141	8.554
1100	19.209	41.735	28.790	14.239	-58.852	-37.166	7.384
1200	19.418	43.415	29.940	16.170	-58.687	-35.164	6.404
1300	19.628	44.978	31.038	18.122	-58.529	-33.199	5.581
1400	19.837	46.440	32.086	20.095	-58.380	-31.267	4.881
1500	20.046	47.816	33.089	22.090	-58.246	-29.331	4.273
1600	20.255	49.116	34.050	24.105	-58.127	-27.397	3.742
1700	20.464	50.350	34.973	26.141	-58.022	-25.471	3.275
1800	20.674	51.526	35.861	28.197	-57.934	-23.565	2.861
1900	20.883	52.649	36.715	30.275	-57.863	-21.684	2.494
2000	21.092	53.726	37.539	32.374	-57.812	-19.763	2.160

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 15.973 + 2.758\times10^{-3}T - 0.592\times10^{5}T^{-2}$

$H°-H°_{298} = 15.973\times10^{-3}T + 1.379\times10^{-6}T^{2} + 0.592\times10^{2}T^{-1} - 5.083$

Formation equations (kcal/mol):

298.15-2000 K: $ΔHf° = -60.902 + 2.322\times10^{-3}T - 0.460\times10^{-6}T^{2} + 104.350T^{-1}$

$ΔGf° = -60.902 - 2.322\times10^{-3}T\ln T + 0.460\times10^{-6}T^{2} + 52.175T^{-1} + 37.153\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Other data are those estimated by Schick (437).

$NbOCl_3(g)$
Niobium Oxide Trichloride (ideal gas)
[Formation: $Nb(c) + 0.5O_2(g) + 1.5Cl_2(g) = NbOCl_3(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	21.954	85.253	85.253	0	-179.800	-171.486	125.701
300	21.984	85.389	85.253	.041	-179.799	-171.433	124.888
400	23.237	91.902	86.132	2.308	-179.732	-168.656	92.148
500	23.990	97.174	87.830	4.672	-179.628	-165.898	72.513
600	24.469	101.594	89.766	7.097	-179.507	-163.161	59.430
700	24.789	105.391	91.734	9.560	-179.383	-160.451	50.094
800	25.011	108.717	93.653	12.051	-179.264	-157.756	43.096
900	25.171	111.672	95.493	14.561	-179.148	-155.070	37.656
1000	25.289	114.331	97.247	17.084	-179.044	-152.403	33.307
1100	25.379	116.745	98.910	19.618	-178.949	-149.744	29.751
1200	25.448	118.957	100.491	22.159	-178.865	-147.075	26.786
1300	25.503	120.996	101.989	24.709	-178.790	-144.421	24.279
1400	25.547	122.887	103.416	27.259	-178.734	-141.786	22.134
1500	25.583	124.651	104.774	29.816	-178.695	-139.147	20.273
1600	25.612	126.303	106.068	32.376	-178.674	-136.506	18.646
1700	25.637	127.857	107.305	34.938	-178.672	-133.865	17.209
1800	25.658	129.323	108.488	37.503	-178.689	-131.233	15.934
1900	25.675	130.710	109.621	40.069	-178.728	-128.606	14.793
2000	25.690	132.028	110.709	42.638	-178.791	-125.959	13.764

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.860 + 0.594\text{x}10^{-3}T - 2.740\text{x}10^{5}T^{-2}$

$H° - H°_{298} = 24.860\text{x}10^{-3}T + 0.297\text{x}10^{-6}T^{2} + 2.740\text{x}10^{2}T^{-1} - 8.357$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -181.130 + 2.809\text{x}10^{-3}T - 0.858\text{x}10^{-6}T^{2} + 169.550T^{-1}$

$\Delta Gf° = -181.130 - 2.809\text{x}10^{-3}T\ln T + 0.858\text{x}10^{-6}T^{2} + 84.775T^{-1} + 47.137\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Other data from Zavalishin (541).

$NbOF_3(g)$
Niobium Oxide Trifluoride (ideal gas)
[Formation: $Nb(c) + 0.5O_2(g) + 1.5F_2(g) = NbOF_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	19.580	76.620	76.620	0	-318.200	-309.480	226.852
300	19.620	76.750	76.623	.038	-318.201	-309.426	225.414
400	21.470	82.670	77.435	2.094	-318.253	-306.499	167.461
500	22.670	87.590	78.992	4.299	-318.234	-303.564	132.686
600	23.480	91.800	80.793	6.604	-318.175	-300.639	109.506
700	24.020	95.470	82.647	8.976	-318.097	-297.737	92.956
800	24.400	98.700	84.462	11.390	-318.019	-294.841	80.546
900	24.680	101.600	86.222	13.840	-317.935	-291.958	70.896
1000	24.890	104.200	87.880	16.320	-317.852	-289.065	63.174
1100	25.050	106.700	89.600	18.810	-317.785	-286.330	56.888
1200	25.160	108.800	91.042	21.310	-317.728	-283.364	51.607
1300	25.260	110.800	92.469	23.830	-317.673	-280.474	47.151
1400	25.330	112.700	93.879	26.350	-317.642	-277.667	43.345
1500	25.400	114.400	95.147	28.880	-317.624	-274.742	40.029
1600	25.450	116.100	96.463	31.420	-317.621	-271.975	37.150
1700	25.490	117.600	97.629	33.950	-317.648	-269.058	34.589
1800	25.530	119.100	98.817	36.510	-317.673	-266.268	32.329
1900	25.570	120.400	99.842	39.060	-317.729	-263.274	30.283
2000	25.580	121.700	100.900	41.600	-317.824	-260.392	28.454

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 23.988 + 1.034\times10^{-3}T - 4.192\times10^{5}T^{-2}$

$H°-H°_{298} = 23.988\times10^{-3}T + 0.517\times10^{-6}T^{2} + 4.192\times10^{2}T^{-1} - 8.604$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -319.745 + 2.415\times10^{-3}T - 0.767\times10^{-6}T^{2} + 266.450T^{-1}$

$\Delta Gf° = -319.745 - 2.415\times10^{-3}T\ln T + 0.767\times10^{-6}T^{2} + 133.225T^{-1} + 46.463\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Alikhanyan (5). Other data from Mendeleeva (330).

$NbSi_2(c)$
Niobium Disilicide
[Formation: $Nb(c) + 2Si(c,l) = NbSi_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°₂₉₈)/T	H°- H°₂₉₈	ΔHf°	ΔGf°	
298.15*	15.440	16.300	16.300	0	-33.000	-32.583	23.883
300	15.450	16.400	16.300	.030	-32.999	-32.579	23.733
400	16.150	20.940	16.915	1.610	-33.033	-32.441	17.725
500	16.660	24.600	18.100	3.250	-33.100	-32.285	14.112
600	17.110	27.680	19.447	4.940	-33.177	-32.115	11.698
700	17.530	30.350	20.821	6.670	-33.262	-31.939	9.972
800	17.930	32.720	22.158	8.450	-33.336	-31.736	8.670
900	18.320	34.850	23.450	10.260	-33.418	-31.528	7.656
1000	18.700	36.800	24.690	12.110	-33.488	-31.298	6.840
1100	19.080	38.600	25.873	14.000	-33.546	-31.093	6.178
1200	19.450	40.280	27.005	15.930	-33.587	-30.851	5.619
1300	19.830	41.850	28.088	17.890	-33.621	-30.618	5.147
1400	20.200	43.330	29.123	19.890	-33.642	-30.380	4.742
1500	20.570	44.740	30.120	21.930	-33.651	-30.171	4.396
1600	20.940	46.080	31.074	24.010	-33.646	-29.934	4.089
1687	21.262	47.197	31.878	25.843	-33.641	-29.688	3.846
1687	21.262	47.197	31.878	25.843	-57.805	-29.688	3.846
1700	21.310	47.360	31.995	26.120	-57.785	-29.463	3.788
1800	21.680	48.590	32.884	28.270	-57.627	-27.801	3.375
1900	22.050	49.770	33.744	30.450	-57.457	-26.164	3.010
2000	22.420	50.910	34.570	32.680	-57.257	-24.517	2.679

*Data 298 to 1000 K estimated.

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 15.096 + 3.670\times10^{-3}T - 0.668\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.096\times10^{-3}T + 1.835\times10^{-6}T^{2} + 0.668\times10^{2}T^{-1} - 4.888$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf^\circ = -32.230 - 1.458\times10^{-3}T + 0.361\times10^{-6}T^{2} - 109.600T^{-1}$

$\Delta Gf^\circ = -32.230 + 1.458\times10^{-3}T\ln T - 0.361\times10^{-6}T^{2} - 54.800T^{-1} - 8.766\times10^{-3}T$

1687-2000 K: $\Delta Hf^\circ = -57.088 - 2.300\times10^{-3}T + 1.063\times10^{-6}T^{2} + 87.400T^{-1}$

$\Delta Gf^\circ = -57.088 + 2.300\times10^{-3}T\ln T - 1.063\times10^{-6}T^{2} + 43.700T^{-1} + 0.862\times10^{-3}T$

Sources: Entropy at 298 K estimated. Other data from Chart (76) who estimated enthalpy of formation at 298 K and heat capacities 298 to 1000 K.

Nb_5Si_3(c)
Pentaniobium Trisilicide
[Formation: $5Nb(c) + 3Si(c,l) = Nb_5Si_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	43.350	57.500	57.500	0	-108.000	-108.149	79.274
300	43.410	57.770	57.503	.080	-108.002	-108.146	78.783
400	45.900	70.630	59.230	4.560	-108.043	-108.199	59.116
500	47.440	81.050	62.590	9.230	-108.086	-108.236	47.309
600	48.620	89.810	66.427	14.030	-108.117	-108.261	39.434
700	49.620	97.380	70.309	18.950	-108.135	-108.296	33.811
800	50.530	104.070	74.120	23.960	-108.160	-108.312	29.589
900	51.380	110.070	77.792	29.050	-108.190	-108.325	26.305
1000	52.200	115.530	81.300	34.230	-108.214	-108.314	23.672
1100	53.000	120.540	84.640	39.490	-108.235	-108.356	21.528
1200	53.780	125.180	87.822	44.830	-108.242	-108.266	19.718
1300	54.560	129.520	90.866	50.250	-108.242	-108.242	18.197
1400	55.320	133.590	93.776	55.740	-108.258	-108.258	16.900
1500	56.080	137.430	96.557	61.310	-108.292	-108.277	15.776
1600	56.840	141.080	99.230	66.960	-108.341	-108.261	14.788
1687	57.493	144.108	101.469	71.932	-108.407	-108.177	14.014
1687	57.493	144.108	101.469	71.932	-144.653	-108.177	14.014
1700	57.590	144.550	101.797	72.680	-144.637	-107.883	13.869
1800	58.340	147.860	104.260	78.480	-144.527	-105.719	12.836
1900	59.080	151.030	106.635	84.350	-144.437	-103.625	11.919
2000	59.830	154.080	108.935	90.290	-144.377	-101.457	11.087

*Data 298 to 1000 K estimated.

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 45.208 + 7.356\times10^{-3}T - 3.604\times10^{5}T^{-2}$

$H°-H°_{298} = 45.208\times10^{-3}T + 3.678\times10^{-6}T^{2} + 3.604\times10^{2}T^{-1} - 15.015$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -109.107 + 2.191\times10^{-3}T - 1.235\times10^{-6}T^{2} + 167.900T^{-1}$

$\Delta Gf° = -109.107 - 2.191\times10^{-3}T\ln T + 1.235\times10^{-6}T^{2} + 83.950T^{-1} + 14.382\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -146.394 + 0.928\times10^{-3}T - 0.182\times10^{-6}T^{2} + 463.400T^{-1}$

$\Delta Gf° = -146.394 - 0.928\times10^{-3}T\ln T + 0.182\times10^{-6}T^{2} + 231.700T^{-1} + 28.825\times10^{-3}T$

Sources: Entropy at 298 K estimated. Other data from Chart (76) who estimated enthalpy of formation at 298 K and heat capacities 298 to 1000 K.

$NdB_6(c)$
Neodymium Hexaboride
[Formation: $Nd(c,l) + 6B(\beta) = NdB_6(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.700	24.730	24.730	0	-72.700	-72.453	53.108
300	23.820	24.880	24.747	.040	-72.701	-72.449	52.778
400	29.180	32.560	25.735	2.730	-72.585	-72.389	39.551
500	32.720	39.470	27.810	5.830	-72.633	-72.328	31.614
600	35.620	45.700	30.283	9.250	-72.808	-72.268	26.323
700	38.220	51.390	32.904	12.940	-73.015	-72.154	22.527
800	40.660	56.650	35.538	16.890	-73.183	-72.007	19.671
900	43.000	61.570	38.159	21.070	-73.319	-71.852	17.448
1000	45.280	66.220	40.730	25.490	-73.395	-71.675	15.664
1100	47.530	70.640	43.249	30.130	-73.419	-71.538	14.213
1128	48.152	71.843	43.944	31.470	-73.416	-71.496	13.852
1128	48.152	71.843	43.944	31.470	-74.140	-71.496	13.852
1200	49.750	74.880	45.722	34.990	-74.070	-71.334	12.992
1289	51.717	78.509	47.858	39.510	-73.880	-71.119	12.058
1289	51.717	78.509	47.858	39.510	-75.587	-71.119	12.058
1300	51.960	78.950	48.119	40.080	-75.555	-71.083	11.950
1400	54.150	82.880	50.466	45.380	-75.195	-70.757	11.046
1500	56.330	86.690	52.750	50.910	-74.695	-70.435	10.262
1600	58.500	90.390	54.984	56.650	-74.075	-70.235	9.594
1700	60.670	94.000	57.171	62.610	-73.319	-70.004	9.000
1800	62.830	97.530	59.319	68.780	-72.437	-69.773	8.471
1900	64.990	100.990	61.427	75.170	-71.419	-69.652	8.012
2000	67.150	104.380	63.490	81.780	-70.265	-69.665	7.613

Phase changes: 1128 K, α - β transition point of Nd; ΔH° = 0.724 kcal/mol.
1289 K, melting point of Nd; ΔH° = 1.707 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.506 + 21.400\text{x}10^{-3}T - 6.211\text{x}10^{5}T\text{-}2$
$H°- H°_{298} = 24.506\text{x}10^{-3}T + 10.700\text{x}10^{-6}T^{2} + 6.211\text{x}10^{2}T^{-1} - 10.341$

Formation equations (kcal/mol):

298.15-1128 K: $\Delta Hf° = -68.561 - 7.800\text{x}10^{-3}T + 3.583\text{x}10^{-6}T^{2} - 635.500T^{-1}$
$\Delta Gf° = -68.561 + 7.800\text{x}10^{-3}T\ln T - 3.583\text{x}10^{-6}T^{2} - 317.750T^{-1} - 52.849\text{x}10^{-3}T$
1128-1289 K: $\Delta Hf° = -65.448 - 14.490\text{x}10^{-3}T + 6.548\text{x}10^{-6}T^{2} - 707.900T^{-1}$
$\Delta Gf° = -65.448 + 14.490\text{x}10^{-3}T\ln T - 6.548\text{x}10^{-6}T^{2} - 353.950T^{-1} - 99.255\text{x}10^{-3}T$
1289-2000 K: $\Delta Hf° = -67.332 - 14.352\text{x}10^{-3}T + 6.548\text{x}10^{-6}T^{2} - 707.900T^{-1}$
$\Delta Gf° = -67.332 + 14.352\text{x}10^{-3}T\ln T - 6.548\text{x}10^{-6}T^{2} - 353.950T^{-1} - 96.805\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Storms (475). Low-temperature heat capacities and entropy at 298 K from Westrum (526). Other data based on Prilepskii (408).

$NdFeO_3(c)$
Neodymium Ferrite
[Formation: $Nd(c) + Fe(c) + 1.5O_2(g) = NdFeO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	25.660	24.000	24.000	0	-326.000	-304.197	222.980
300	25.680	24.160	24.000	.050	-325.992	-304.058	221.504
400	27.290	31.760	25.010	2.700	-325.704	-296.785	162.154
500	29.100	38.040	27.020	5.510	-325.379	-289.602	126.583
600	30.980	43.510	29.310	8.520	-324.984	-282.473	102.889
700	32.890	48.430	31.701	11.710	-324.544	-275.422	85.990
800	34.830	52.950	34.075	15.100	-324.059	-268.439	73.333
900	36.770	57.160	36.404	18.680	-323.564	-261.513	63.503
1000	38.720	61.140	38.690	22.450	-323.138	-254.653	55.654

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 18.950 + 19.700\text{x}10^{-3}T + 0.740\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 18.950\text{x}10^{-3}T + 9.850\text{x}10^{-6}T^{2} - 0.740\text{x}10^{2}T^{-1} - 6.277$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -327.838 + 4.358\text{x}10^{-3}T + 0.060\text{x}10^{-6}T^{2} + 159.100T^{-1}$

$\Delta Gf° = -327.838 - 4.358\text{x}10^{-3}T\ln T - 0.060\text{x}10^{-6}T^{2} + 79.550T^{-1} + 103.246\text{x}10^{-3}T$

Source: Data based on Kaul (237).

NdO(g)
Neodymium Monoxide (ideal gas)
[Formation: $Nd(c,l) + 0.5O_2(g) = NdO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.570	60.520	60.520	0	-30.000	-35.640	26.125
300	7.580	60.568	60.521	.014	-30.003	-35.675	25.989
400	7.950	62.800	60.822	.791	-30.253	-37.527	20.504
500	8.220	64.604	61.404	1.600	-30.516	-39.318	17.186
600	8.400	66.120	62.067	2.432	-30.807	-41.049	14.952
700	8.520	67.425	62.742	3.278	-31.139	-42.728	13.340
800	8.610	68.569	63.400	4.135	-31.523	-44.362	12.119
900	8.670	69.588	64.032	5.000	-31.966	-45.942	11.156
1000	8.720	70.504	64.634	5.870	-32.478	-47.467	10.374
1100	8.760	71.337	65.206	6.744	-33.063	-48.939	9.723
1128	8.766	71.557	65.361	6.989	-33.241	-49.346	9.561
1128	8.766	71.557	65.361	6.989	-33.965	-49.346	9.561
1200	8.780	72.101	65.750	7.621	-34.408	-50.316	9.164
1289	8.807	72.728	66.209	8.403	-34.954	-51.480	8.728
1289	8.807	72.728	66.209	8.403	-36.661	-51.480	8.728
1300	8.810	72.803	66.265	8.500	-36.728	-51.608	8.676
1400	8.820	73.457	66.756	9.382	-37.330	-52.730	8.231
1500	8.840	74.067	67.224	10.265	-37.934	-53.819	7.841
1600	8.850	74.638	67.669	11.150	-38.539	-54.857	7.493
1700	8.860	75.175	68.095	12.036	-39.146	-55.854	7.180
1800	8.870	75.682	68.503	12.922	-39.756	-56.822	6.899
1900	8.880	76.161	68.893	13.809	-40.368	-57.750	6.643
2000	8.880	76.617	69.268	14.697	-40.982	-58.649	6.409

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1128 K, α - β transition point of Nd; ΔH° = 0.724 kcal/mol.
1289 K, melting point of Nd; ΔH° = 1.707 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.447 + 0.302\times10^{-3}T - 0.860\times10^{5}T^{-2}$

$H°-H°_{298} = 8.447\times10^{-3}T + 0.151\times10^{-6}T^{2} + 0.860\times10^{2}T^{-1} - 2.820$

Formation equations (kcal/mol):

298.15-1128 K: $\Delta Hf° = -30.441 + 0.864\times10^{-3}T - 3.066\times10^{-6}T^{2} + 135.800T^{-1}$

$\Delta Gf° = -30.441 - 0.864\times10^{-3}T\ln T + 3.066\times10^{-6}T^{2} + 67.900T^{-1} - 14.195\times10^{-3}T$

1128-1289 K: $\Delta Hf° = -27.327 - 5.826\times10^{-3}T - 0.100\times10^{-6}T^{2} + 63.400T^{-1}$

$\Delta Gf° = -27.327 + 5.826\times10^{-3}T\ln T + 0.100\times10^{-6}T^{2} + 31.700T^{-1} - 60.601\times10^{-3}T$

1289-2000 K: $\Delta Hf° = -29.212 - 5.688\times10^{-3}T - 0.100\times10^{-6}T^{2} + 63.400T^{-1}$

$\Delta Gf° = -29.212 + 5.688\times10^{-3}T\ln T + 0.100\times10^{-6}T^{2} + 31.700T^{-1} - 58.151\times10^{-3}T$

Source: Data from Pedley (396) who estimated all except enthalpy of formation at 298 K.

$NdPO_4(c)$
Neodymium Phosphate
[Formation: $Nd(c,l) + P(c,l,1/4P_4(g)) + 2O_2(g) = NdPO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	24.950	25.800	25.800	0	-453.000	-423.444	310.389
300	25.050	25.950	25.800	.046	-453.002	-423.259	308.340
317.3	25.716	27.373	25.844	.485	-453.019	-421.542	290.346
317.3	25.716	27.373	25.844	.485	-453.176	-421.542	290.346
400	28.900	33.750	26.837	2.765	-453.151	-413.299	225.813
500	31.150	40.460	28.910	5.775	-452.938	-403.360	176.306
550	31.965	43.473	30.098	7.356	-452.788	-398.421	158.316
550	31.965	43.473	30.098	7.356	-455.696	-398.421	158.316
600	32.780	46.290	31.332	8.975	-455.449	-393.225	143.230
700	34.110	51.440	33.839	12.321	-454.920	-382.888	119.541
800	35.280	56.070	36.330	15.792	-454.365	-372.638	101.799
900	36.360	60.290	38.763	19.374	-453.795	-362.459	88.016
1000	37.380	64.180	41.119	23.061	-453.215	-352.347	77.004
1100	38.360	67.790	43.382	26.849	-452.632	-342.289	68.006
1128	38.629	68.758	44.000	27.927	-452.469	-339.487	65.775
1128	38.629	68.758	44.000	27.927	-453.193	-339.487	65.775
1200	39.320	71.170	45.559	30.733	-452.730	-332.246	60.510
1289	40.166	74.008	47.421	34.271	-452.099	-323.333	54.820
1289	40.166	74.008	47.421	34.271	-453.806	-323.333	54.820
1300	40.270	74.350	47.648	34.713	-453.723	-322.221	54.170
1400	41.200	77.370	49.666	38.786	-452.921	-312.138	48.726
1500	42.110	80.240	51.605	42.952	-452.039	-302.117	44.018
1600	43.030	82.990	53.484	47.209	-451.080	-292.155	39.906

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.
1128 K, α - β transition point of Nd; ΔH° = 0.724 kcal/mol.
1289 K, melting point of Nd; ΔH° = 1.707 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 29.197 + 8.794\times10^{-3}T - 6.102\times10^{5}T^{-2}$
$H°-H°_{298} = 29.197\times10^{-3}T + 4.397\times10^{-6}T^2 + 6.102\times10^{2}T^{-1} - 11.143$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -456.819 + 6.970\times10^{-3}T - 2.759\times10^{-6}T^2 + 592.200T^{-1}$
$\Delta Gf° = -456.819 - 6.970\times10^{-3}T\ln T + 2.759\times10^{-6}T^2 + 296.100T^{-1} + 147.498\times10^{-3}T$
317.3-550 K: $\Delta Hf° = -456.506 + 4.477\times10^{-3}T + 0.426\times10^{-6}T^2 + 592.200T^{-1}$
$\Delta Gf° = -456.506 - 4.477\times10^{-3}T\ln T - 0.426\times10^{-6}T^2 + 296.100T^{-1} + 133.162\times10^{-3}T$
550-1128 K: $\Delta Hf° = -459.966 + 5.815\times10^{-3}T + 0.422\times10^{-6}T^2 + 491.900T^{-1}$
$\Delta Gf° = -459.966 - 5.815\times10^{-3}T\ln T - 0.422\times10^{-6}T^2 + 245.950T^{-1} + 148.059\times10^{-3}T$
1128-1289 K: $\Delta Hf° = -456.852 - 0.875\times10^{-3}T + 3.387\times10^{-6}T^2 + 419.500T^{-1}$
$\Delta Gf° = -456.852 + 0.875\times10^{-3}T\ln T - 3.387\times10^{-6}T^2 + 209.750T^{-1} + 101.653\times10^{-3}T$
1289-1600 K: $\Delta Hf° = -458.737 - 0.737\times10^{-3}T + 3.387\times10^{-6}T^2 + 419.500T^{-1}$
$\Delta Gf° = -458.737 + 0.737\times10^{-3}T\ln T - 3.387\times10^{-6}T^2 + 209.750T^{-1} + 104.104\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Ashuiko (13). Other data based on Tsagareishvili (504).

$NiAl_2Cl_8(g)$
Nickel Aluminum Chloride (ideal gas)
[Formation: $Ni(c) + 2Al(c,l) + 4Cl_2(g) = NiAl_2Cl_8(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	53.966	146.000	146.000	0	-369.000	-342.807	251.281
300	54.045	146.334	146.001	.100	-368.994	-342.645	249.613
400	57.058	162.345	148.163	5.673	-368.589	-333.923	182.445
500	58.652	175.265	152.333	11.466	-368.166	-325.303	142.188
600	59.603	186.049	157.079	17.382	-367.810	-316.766	115.381
631	59.802	189.057	158.577	19.233	-367.730	-314.129	108.799
700	60.244	195.288	161.894	23.376	-367.490	-308.278	96.248
800	60.741	203.366	166.583	29.426	-367.159	-299.850	81.914
900	61.186	210.546	171.077	35.522	-366.891	-291.453	70.774
933.61	61.337	212.792	172.539	37.581	-366.817	-288.636	67.566
933.61	61.337	212.792	172.539	37.581	-371.977	-288.636	67.566
1000	61.635	217.015	175.352	41.663	-371.788	-282.723	61.788

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 59.699 + 2.442\times10^{-3}T - 5.743\times10^{5}T^{-2}$
$H° - H°_{298} = 59.699\times10^{-3}T + 1.221\times10^{-6}T^{2} + 5.743\times10^{2}T^{-1} - 19.834$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -373.355 + 12.211\times10^{-3}T - 6.865\times10^{-6}T^{2} + 394.900T^{-1}$
$\Delta Gf° = -373.355 - 12.211\times10^{-3}T\ln T + 6.865\times10^{-6}T^{2} + 197.450T^{-1} + 167.764\times10^{-3}T$
631-750 K: $\Delta Hf° = -370.806 + 3.887\times10^{-3}T + 0.160\times10^{-6}T^{2} + 335.900T^{-1}$
$\Delta Gf° = -370.806 - 3.887\times10^{-3}T\ln T - 0.160\times10^{-6}T^{2} + 167.950T^{-1} + 114.564\times10^{-3}T$
750-933.61 K: $\Delta Hf° = -373.716 + 10.136\times10^{-3}T - 3.742\times10^{-6}T^{2} + 649.500T^{-1}$
$\Delta Gf° = -373.716 - 10.136\times10^{-3}T\ln T + 3.742\times10^{-6}T^{2} + 324.750T^{-1} + 156.608\times10^{-3}T$
933.61-1000 K: $\Delta Hf° = -376.251 + 4.140\times10^{-3}T - 0.288\times10^{-6}T^{2} + 614.700T^{-1}$
$\Delta Gf° = -376.251 - 4.140\times10^{-3}T\ln T + 0.288\times10^{-6}T^{2} + 307.350T^{-1} + 121.561\times10^{-3}T$

Source: Data from Mah (320) who estimated all except enthalpy of formation and entropy at 298 K.

$NiAl_2O_4$(c)
Nickel Aluminate
[Formation: Ni(c) + 2Al(c,l) + $2O_2$(g) = $NiAl_2O_4$(c)]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	29.530	21.000	21.000	0	-463.500	-434.370	318.398
300	29.560	21.180	21.013	.050	-463.510	-434.193	316.306
400	31.120	29.900	22.175	3.090	-463.738	-424.382	231.869
500	32.610	37.010	24.450	6.280	-463.968	-414.515	181.182
600	34.070	43.080	27.063	9.610	-464.232	-404.602	147.374
631	34.520	44.808	27.893	10.673	-464.332	-401.516	139.065
700	35.520	48.440	29.740	13.090	-464.470	-394.635	123.209
800	36.960	53.280	32.392	16.710	-464.621	-384.661	105.083
900	38.400	57.710	34.954	20.480	-464.747	-374.652	90.977
933.61	38.881	59.127	35.799	21.779	-464.786	-371.286	86.914
933.61	38.881	59.127	35.799	21.779	-469.946	-371.286	86.914
1000	39.830	61.830	37.440	24.390	-469.953	-364.275	79.611
1100	41.270	65.700	39.836	28.450	-469.867	-353.703	70.273

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp^\circ = 25.560 + 14.300\text{x}10^{-3}T - 0.260\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 25.560\text{x}10^{-3}T + 7.150\text{x}10^{-6}T^2 + 0.260\text{x}10^{2}T^{-1} - 8.344$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -463.135 - 1.080\text{x}10^{-3}T - 1.590\text{x}10^{-6}T^2 + 29.400T^{-1}$
$\Delta Gf^\circ = -463.135 + 1.080\text{x}10^{-3}T\ln T + 1.590\text{x}10^{-6}T^2 + 14.700T^{-1} + 89.686\text{x}10^{-3}T$
631-750 K: $\Delta Hf^\circ = -460.586 - 9.404\text{x}10^{-3}T + 5.435\text{x}10^{-6}T^2 - 29.600T^{-1}$
$\Delta Gf^\circ = -460.586 + 9.404\text{x}10^{-3}T\ln T - 5.435\text{x}10^{-6}T^2 - 14.800T^{-1} + 36.486\text{x}10^{-3}T$
750-933.61 K: $\Delta Hf^\circ = -463.496 - 3.155\text{x}10^{-3}T + 1.533\text{x}10^{-6}T^2 + 284.000T^{-1}$
$\Delta Gf^\circ = -463.496 + 3.155\text{x}10^{-3}T\ln T - 1.533\text{x}10^{-6}T^2 + 142.000T^{-1} + 78.530\text{x}10^{-3}T$
933.61-1100 K: $\Delta Hf^\circ = -466.032 - 9.151\text{x}10^{-3}T + 4.987\text{x}10^{-6}T^2 + 249.200T^{-1}$
$\Delta Gf^\circ = -466.032 + 9.151\text{x}10^{-3}T\ln T - 4.987\text{x}10^{-6}T^2 + 124.600T^{-1} + 43.483\text{x}10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Levitskii (305) and Mah (320). Other data based on Chizhikov (91).

NiB(c)
Nickel Boride
[Formation: Ni(c) + B(β) = NiB(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.280	6.800	6.800	0	-11.100	-10.578	7.754
300	8.330	6.850	6.800	.020	-11.097	-10.569	7.699
400	9.990	9.500	7.150	.940	-11.146	-10.394	5.679
500	10.940	11.840	7.860	1.990	-11.213	-10.198	4.457
600	11.620	13.900	8.700	3.120	-11.340	-9.990	3.639
631	11.790	14.490	8.970	3.483	-11.403	-9.917	3.435
700	12.170	15.730	9.573	4.310	-11.466	-9.744	3.042
800	12.650	17.390	10.452	5.550	-11.509	-9.501	2.596
900	13.090	18.900	11.300	6.840	-11.536	-9.241	2.244
1000	13.500	20.300	12.130	8.170	-11.556	-8.986	1.964
1100	13.900	21.610	12.937	9.540	-11.568	-8.730	1.734
1200	14.280	22.840	13.715	10.950	-11.573	-8.477	1.544
1300	14.660	23.990	14.459	12.390	-11.582	-8.215	1.381

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp° = 10.268 + 3.502\times10^{-3}T - 2.692\times10^{5}T^{-2}$

$H°-H°_{298} = 10.268\times10^{-3}T + 1.751\times10^{-6}T^{2} + 2.692\times10^{2}T^{-1} - 4.120$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -11.932 + 2.549\times10^{-3}T - 3.221\times10^{-6}T^{2} + 106.700T^{-1}$

$\Delta Gf° = -11.932 - 2.549\times10^{-3}T\ln T + 3.221\times10^{-6}T^{2} + 53.350T^{-1} + 17.502\times10^{-3}T$

631-750 K: $\Delta Hf° = -9.383 - 5.775\times10^{-3}T + 3.804\times10^{-6}T^{2} + 47.700T^{-1}$

$\Delta Gf° = -9.383 + 5.775\times10^{-3}T\ln T - 3.804\times10^{-6}T^{2} + 23.850T^{-1} - 35.698\times10^{-3}T$

750-1300 K: $\Delta Hf° = -12.293 + 0.474\times10^{-3}T - 0.098\times10^{-6}T^{2} + 361.300T^{-1}$

$\Delta Gf° = -12.293 - 0.474\times10^{-3}T\ln T + 0.098\times10^{-6}T^{2} + 180.650T^{-1} + 6.345\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Sato (435). Other data from Hack (200) who estimated all except entropy at 298 K.

$Ni_2B(c)$
Dinickel Boride
[Formation: $2Ni(c) + B(\beta) = Ni_2B(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.320	15.860	15.860	0	-15.230	-15.281	11.201
300	14.370	15.950	15.860	.030	-15.229	-15.277	11.129
400	16.300	20.380	16.455	1.570	-15.310	-15.290	8.354
500	17.480	24.150	17.630	3.260	-15.447	-15.272	6.675
600	18.360	27.420	18.987	5.060	-15.686	-15.218	5.543
631	18.593	28.351	19.424	5.633	-15.808	-15.187	5.260
700	19.110	30.300	20.400	6.930	-15.930	-15.104	4.716
800	19.770	32.900	21.800	8.880	-16.000	-14.984	4.093
900	20.400	35.270	23.170	10.890	-16.055	-14.858	3.608
1000	21.000	37.450	24.490	12.960	-16.097	-14.727	3.219
1100	21.580	39.480	25.771	15.080	-16.137	-14.586	2.898
1200	22.150	41.380	26.988	17.270	-16.158	-14.442	2.630
1300	22.710	43.170	28.162	19.510	-16.182	-14.297	2.404
1398	23.250	44.840	29.268	21.770	-16.193	-14.143	2.211

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1398 K, melting point of Ni_2B; ΔH° = 10.07 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1398 K: $Cp° = 15.982 + 5.304\times10^{-3}T - 2.882\times10^{5}T^{-2}$
$H°-H°_{298} = 15.982\times10^{-3}T + 2.652\times10^{-6}T^{2} + 2.882\times10^{2}T^{-1} - 5.967$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -16.833 + 5.267\times10^{-3}T - 6.600\times10^{-6}T^{2} + 184.700T^{-1}$
$\Delta Gf° = -16.833 - 5.267\times10^{-3}T\ln T + 6.600\times10^{-6}T^{2} + 92.350T^{-1} + 32.210\times10^{-3}T$
631-750 K: $\Delta Hf° = -11.735 - 11.381\times10^{-3}T + 7.450\times10^{-6}T^{2} + 66.700T^{-1}$
$\Delta Gf° = -11.735 + 11.381\times10^{-3}T\ln T - 7.450\times10^{-6}T^{2} + 33.350T^{-1} - 74.190\times10^{-3}T$
750-1398 K: $\Delta Hf° = -17.555 + 1.117\times10^{-3}T - 0.354\times10^{-6}T^{2} + 693.900T^{-1}$
$\Delta Gf° = -17.555 - 1.117\times10^{-3}T\ln T + 0.354\times10^{-6}T^{2} + 346.950T^{-1} + 9.897\times10^{-3}T$

Source: Data from Hack (200) who estimated all except enthalpy of formation and entropy at 298 K.

$Ni_3B(c)$
Trinickel Boride
[Formation: $3Ni(c) + B(\beta) = Ni_3B(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	20.470	21.000	21.000	0	-21.260	-20.714	15.184
300	20.540	21.130	21.000	.040	-21.261	-20.709	15.086
400	22.980	27.410	21.835	2.230	-21.344	-20.516	11.209
500	24.450	32.700	23.500	4.600	-21.511	-20.296	8.871
600	25.530	37.260	25.427	7.100	-21.832	-20.038	7.299
631	25.812	38.553	26.040	7.896	-22.000	-19.936	6.905
700	26.440	41.260	27.403	9.700	-22.144	-19.687	6.146
800	27.240	44.850	29.362	12.390	-22.211	-19.339	5.283
900	28.000	48.100	31.267	15.150	-22.264	-18.979	4.609
1000	28.710	51.090	33.100	17.990	-22.298	-18.618	4.069
1100	29.410	53.860	34.869	20.890	-22.336	-18.233	3.623
1200	30.090	56.440	36.548	23.870	-22.363	-17.851	3.251
1300	30.760	58.880	38.180	26.910	-22.402	-17.488	2.940
1400	31.420	61.180	39.737	30.020	-22.445	-17.097	2.669
1439	31.670	62.050	40.334	31.250	-22.467	-16.953	2.575

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1439 K, melting point of Ni_3B; ΔH° = 17.28 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1439 K: $Cp^\circ = 22.782 + 6.304\times10^{-3}T - 3.722\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 22.782\times10^{-3}T + 3.152\times10^{-6}T^{2} + 3.722\times10^{2}T^{-1} - 8.321$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -24.141 + 9.071\times10^{-3}T - 10.380\times10^{-6}T^{2} + 327.700T^{-1}$
$\Delta Gf^\circ = -24.141 - 9.071\times10^{-3}T\ln T + 10.380\times10^{-6}T^{2} + 163.850T^{-1} + 58.238\times10^{-3}T$
631-750 K: $\Delta Hf^\circ = -16.494 - 15.901\times10^{-3}T + 10.695\times10^{-6}T^{2} + 150.700T^{-1}$
$\Delta Gf^\circ = -16.494 + 15.901\times10^{-3}T\ln T - 10.695\times10^{-6}T^{2} + 75.350T^{-1} - 101.362\times10^{-3}T$
750-1439 K: $\Delta Hf^\circ = -25.224 + 2.846\times10^{-3}T - 1.011\times10^{-6}T^{2} + 1091.500T^{-1}$
$\Delta Gf^\circ = -25.224 - 2.846\times10^{-3}T\ln T + 1.011\times10^{-6}T^{2} + 545.750T^{-1} + 24.769\times10^{-3}T$

Source: Data from Hack (200) who estimated all except enthalpy of formation and entropy at 298 K.

$Ni_{3.95}B_{3.05}$(monoclinic)

Monoclinic Tetranickel Triboride

[Formation: $3.95Ni(c) + 3.05B(\beta) = Ni_{3.95}B_{3.05}(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	30.670	33.500	33.500	0	-42.900	-43.197	31.664
300	30.820	33.690	33.500	.060	-42.903	-43.193	31.466
400	36.390	43.410	34.785	3.450	-43.055	-43.277	23.645
500	39.600	51.900	37.380	7.260	-43.291	-43.306	18.929
600	41.880	59.330	40.430	11.340	-43.748	-43.285	15.766
631	42.450	61.454	41.411	12.647	-43.981	-43.248	14.979
700	43.720	65.930	43.616	15.620	-44.200	-43.143	13.470
800	45.330	71.870	46.783	20.070	-44.327	-42.992	11.745
900	46.800	77.300	49.878	24.680	-44.407	-42.825	10.399
1000	48.190	82.300	52.870	29.430	-44.460	-42.652	9.321
1100	49.520	86.950	55.750	34.320	-44.486	-42.440	8.432
1200	50.820	91.320	58.545	39.330	-44.508	-42.273	7.699
1300	52.090	95.440	61.225	44.480	-44.511	-42.086	7.075

*Data except enthalpy of formation at 298 K estimated.

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 37.326 + 11.766\times10^{-3}T - 9.034\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 37.326\times10^{-3}T + 5.883\times10^{-6}T^{2} + 9.034\times10^{2}T^{-1} - 14.682$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -46.584 + 11.087\times10^{-3}T - 13.134\times10^{-6}T^{2} + 460.875T^{-1}$

$\Delta Gf^\circ = -46.584 - 11.087\times10^{-3}T\ln T + 13.134\times10^{-6}T^{2} + 230.438T^{-1} + 68.018\times10^{-3}T$

631-750 K: $\Delta Hf^\circ = -36.516 - 21.793\times10^{-3}T + 14.615\times10^{-6}T^{2} + 227.825T^{-1}$

$\Delta Gf^\circ = -36.516 + 21.793\times10^{-3}T\ln T - 14.615\times10^{-6}T^{2} + 113.913T^{-1} - 142.122\times10^{-3}T$

750-1300 K: $\Delta Hf^\circ = -48.010 + 2.890\times10^{-3}T - 0.798\times10^{-6}T^{2} + 1466.545T^{-1}$

$\Delta Gf^\circ = -48.010 - 2.890\times10^{-3}T\ln T + 0.798\times10^{-6}T^{2} + 733.273T^{-1} + 23.951\times10^{-3}T$

Source: Data from Hack (200) who estimated all except enthalpy of formation at 298 K.

$Ni_{4.1}B_{2.9}$(orthorhombic)

Orthorhombic Tetranickel Triboride
[Formation: $4.1Ni(c) + 2.9B(\beta) = Ni_{4.1}B_{2.9}(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	30.670	34.300	34.300	0.	-42.800	-43.079	31.578
300	30.820	34.490	34.300	.060	-42.804	-43.075	31.380
400	36.390	44.210	35.585	3.450	-43.006	-43.145	23.573
500	39.590	52.700	38.180	7.260	-43.288	-43.148	18.860
600	41.880	60.130	41.230	11.340	-43.791	-43.092	15.696
631	42.450	62.254	42.211	12.647	-44.040	-43.042	14.908
700	43.720	66.720	44.406	15.620	-44.285	-42.900	13.394
800	45.330	72.670	47.583	20.070	-44.440	-42.709	11.667
900	46.800	78.090	50.668	24.680	-44.547	-42.482	10.316
1000	48.190	83.100	53.670	29.430	-44.627	-42.264	9.237
1100	49.520	87.750	56.550	34.320	-44.678	-41.993	8.343
1200	50.820	92.120	59.345	39.330	-44.727	-41.768	7.607

*Data except enthalpy of formation at 298 K estimated.

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 37.326 + 11.766\times10^{-3}T - 9.034\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 37.326\times10^{-3}T + 5.883\times10^{-6}T^{2} + 9.034\times10^{2}T^{-1} - 14.682$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -46.654 + 11.346\times10^{-3}T - 13.672\times10^{-6}T^{2} + 502.950T^{-1}$
$\Delta Gf^\circ = -46.654 - 11.346\times10^{-3}T\ln T + 13.672\times10^{-6}T^{2} + 251.475T^{-1} + 69.728\times10^{-3}T$
631-750 K: $\Delta Hf^\circ = -36.204 - 22.783\times10^{-3}T + 15.131\times10^{-6}T^{2} + 261.050T^{-1}$
$\Delta Gf^\circ = -36.204 + 22.783\times10^{-3}T\ln T - 15.131\times10^{-6}T^{2} + 130.525T^{-1} - 148.391\times10^{-3}T$
750-1200 K: $\Delta Hf^\circ = -48.135 + 2.838\times10^{-3}T - 0.867\times10^{-6}T^{2} + 1546.810T^{-1}$
$\Delta Gf^\circ = -48.135 - 2.838\times10^{-3}T\ln T + 0.867\times10^{-6}T^{2} + 773.405T^{-1} + 23.987\times10^{-3}T$

Source: Data from Hack (200) who estimated all except enthalpy of formation at 298 K.

$Ni_3C(c)$
Trinickel Carbide
[Formation: $3Ni(c) + C(c) = Ni_3C(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$ΔHf°$	$ΔGf°$	
298.15*	25.491	25.400	25.400	0	9.000	8.222	-6.027
300	25.500	25.558	25.401	.047	9.007	8.217	-5.986
400	26.000	32.962	26.407	2.622	9.382	7.890	-4.311
500	26.500	38.818	28.324	5.247	9.560	7.490	-3.274
600	27.000	43.693	30.490	7.922	9.512	7.071	-2.575
631	27.155	45.057	31.172	8.761	9.418	6.952	-2.408
700	27.500	47.893	32.683	10.647	9.419	6.691	-2.089
800	28.000	51.598	34.820	13.422	9.524	6.285	-1.717

*Data except enthalpy of formation at 298 K estimated.

Phase change: 631 K, Curie temperature of Ni; $ΔH° = 0$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 24.000 + 5.000\times10^{-3}T$

$H°-H°_{298} = 24.000\times10^{-3}T + 2.500\times10^{-6}T^2 - 7.378$

Formation equations (kcal/mol):

298.15-631 K: $ΔHf° = 6.545 + 11.494\times10^{-3}T - 11.106\times10^{-6}T^2 + 4.700T^{-1}$

$ΔGf° = 6.545 - 11.494\times10^{-3}T\ln T + 11.106\times10^{-6}T^2 + 2.350T^{-1} + 67.778\times10^{-3}T$

631-750 K: $ΔHf° = 14.191 - 13.478\times10^{-3}T + 9.969\times10^{-6}T^2 - 172.300T^{-1}$

$ΔGf° = 14.191 + 13.478\times10^{-3}T\ln T - 9.969\times10^{-6}T^2 - 86.150T^{-1} - 91.822\times10^{-3}T$

750-800 K: $ΔHf° = 5.461 + 5.269\times10^{-3}T - 1.737\times10^{-6}T^2 + 768.500T^{-1}$

$ΔGf° = 5.461 - 5.269\times10^{-3}T\ln T + 1.737\times10^{-6}T^2 + 384.250T^{-1} + 34.309\times10^{-3}T$

Source: Data from Barin (23) who estimated all except enthalpy of formation at 298 K.

$Ni(CO)_4(g)$

Nickel Tetracarbonyl (ideal gas)

[Formation: $Ni(c) + 4C(c) + 2O_2(g) = Ni(CO)_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	35.681	99.327	99.327	0	-138.300	-134.928	98.903
300	35.745	99.548	99.328	.066	-138.288	-134.907	98.278
400	38.331	110.219	100.764	3.782	-137.620	-133.883	73.149
500	40.031	118.964	103.556	7.704	-137.138	-133.010	58.138
600	41.388	126.387	106.759	11.777	-136.865	-132.213	48.158
631	41.759	128.481	107.775	13.065	-136.830	-131.972	45.709
700	42.540	132.855	110.034	15.975	-136.717	-131.445	41.039
800	43.524	138.602	113.253	20.279	-136.582	-130.707	35.707
900	44.358	143.778	116.361	24.675	-136.510	-129.981	31.563
1000	45.060	148.489	119.343	29.146	-136.483	-129.262	28.250

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 37.436 + 8.238 \times 10^{-3}T - 3.743 \times 10^{5}T^{-2}$

$H° - H°_{298} = 37.436 \times 10^{-3}T + 4.119 \times 10^{-6}T^{2} + 3.743 \times 10^{2}T^{-1} - 12.783$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -138.524 + 5.908 \times 10^{-3}T - 4.231 \times 10^{-6}T^{2} - 346.300T^{-1}$

$\Delta Gf° = -138.524 - 5.908 \times 10^{-3}T\ln T + 4.231 \times 10^{-6}T^{2} - 173.150T^{-1} + 46.410 \times 10^{-3}T$

631-750 K: $\Delta Hf° = -135.975 - 2.416 \times 10^{-3}T + 2.794 \times 10^{-6}T^{2} - 405.300T^{-1}$

$\Delta Gf° = -135.975 + 2.416 \times 10^{-3}T\ln T - 2.794 \times 10^{-6}T^{2} - 202.650T^{-1} - 6.790 \times 10^{-3}T$

750-1000 K: $\Delta Hf° = -138.885 + 3.833 \times 10^{-3}T - 1.108 \times 10^{-6}T^{2} - 91.700T^{-1}$

$\Delta Gf° = -138.885 - 3.833 \times 10^{-3}T\ln T + 1.108 \times 10^{-6}T^{2} - 45.850T^{-1} + 35.253 \times 10^{-3}T$

Source: Data from Mah (320).

$NiFe_2Cl_8(g)$
Nickel Iron Chloride (ideal gas)
[Formation: $Ni(c) + 2Fe(c) + 4Cl_2(g) = NiFe_2Cl_8(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	56.759	170.000	170.000	0	-215.000	-196.115	143.754
300	56.816	170.351	170.001	.105	-214.989	-195.998	142.783
400	58.944	187.026	172.261	5.906	-214.412	-189.759	103.678
500	60.002	200.305	176.587	11.859	-213.945	-183.652	80.273
600	60.599	211.302	181.482	17.892	-213.644	-177.625	64.699
631	60.722	214.358	183.023	19.772	-213.599	-175.763	60.876
700	60.996	220.675	186.429	23.972	-213.464	-171.631	53.585
800	61.323	228.841	191.230	30.089	-213.358	-165.671	45.259
900	61.653	236.083	195.820	36.237	-213.442	-159.706	38.781
1000	62.029	242.597	200.176	42.421	-213.868	-153.723	33.596

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 60.921 + 1.360\times10^{-3}T - 4.060\times10^{5}T^{-2}$

$H°- H°_{298} = 60.921\times10^{-3}T + 0.680\times10^{-6}T^{2} + 4.060\times10^{2}T^{-1} - 19.586$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -222.620 + 23.059\times10^{-3}T - 16.094\times10^{-6}T^{2} + 648.800T^{-1}$

$\Delta Gf° = -222.620 - 23.059\times10^{-3}T\ln T + 16.094\times10^{-6}T^{2} + 324.400T^{-1} + 211.832\times10^{-3}T$

631-750 K: $\Delta Hf° = -220.072 + 14.735\times10^{-3}T - 9.069\times10^{-6}T^{2} + 589.800T^{-1}$

$\Delta Gf° = -220.072 - 14.735\times10^{-3}T\ln T + 9.069\times10^{-6}T^{2} + 294.900T^{-1} + 158.632\times10^{-3}T$

750-1000 K: $\Delta Hf° = -222.982 + 20.984\times10^{-3}T - 12.971\times10^{-6}T^{2} + 903.400T^{-1}$

$\Delta Gf° = -222.982 - 20.984\times10^{-3}T\ln T + 12.971\times10^{-6}T^{2} + 451.700T^{-1} + 200.676\times10^{-3}T$

Source: Data from Mah (320) who estimated all except enthalpy of formation and entropy at 298 K.

$NiFe_2O_4(c)$
Nickel Ferrite
[Formation: $Ni(c,l) + 2Fe(c) + 2O_2(g) = NiFe_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	34.813	30.702	30.702	0	-255.300	-229.215	168.017
300	34.896	30.918	30.705	.064	-255.296	-229.054	166.863
400	40.266	41.745	32.142	3.841	-254.843	-220.366	120.401
500	43.898	51.143	35.025	8.059	-254.161	-211.823	92.587
600	46.798	59.406	38.413	12.596	-253.390	-203.428	74.098
631	47.785	61.788	39.503	14.062	-253.151	-200.851	69.565
700	49.983	66.849	41.952	17.428	-252.502	-195.162	60.931
800	54.616	73.802	45.501	22.641	-251.352	-187.051	51.099
880	60.263	79.256	48.322	27.222	-250.186	-180.675	44.870
880	48.500	79.256	48.322	27.222	-250.186	-180.675	44.870
900	48.500	80.346	49.022	28.192	-250.101	-179.096	43.490
1000	48.500	85.456	52.414	33.042	-249.939	-171.225	37.421
1043	48.500	87.498	53.819	35.127	-250.173	-167.837	35.168
1100	48.500	90.078	55.631	37.892	-250.209	-163.322	32.449
1185	48.500	93.688	58.233	42.014	-249.970	-156.620	28.885
1185	48.500	93.688	58.233	42.014	-250.400	-156.620	28.885
1200	48.500	94.298	58.680	42.742	-250.293	-155.435	28.308
1300	48.500	98.180	61.571	47.592	-249.610	-147.560	24.807
1400	48.500	101.774	64.315	52.442	-249.005	-139.732	21.813
1500	48.500	105.12[illegible]	66.926	57.292	-248.474	-131.950	19.225
1600	48.500	108.251	69.412	62.142	-248.020	-124.191	16.964
1667	48.500	110.240	71.013	65.391	-247.756	-119.023	15.604
1667	48.500	110.240	71.013	65.391	-248.156	-119.023	15.604
1700	48.500	111.191	71.784	66.992	-248.090	-116.467	14.973
1728	48.500	111.983	72.429	68.350	-248.041	-114.285	14.454
1728	48.500	111.983	72.429	68.350	-252.141	-114.285	14.454
1800	48.500	113.963	74.051	71.842	-252.043	-108.542	13.179

*Zero point entropy estimated.

Phase changes:
631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
880 K, α - β transition point of $NiFe_2O_4$; ΔH° = 0 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-880 K: $Cp° = 29.936 + 31.136\times10^{-3}T - 3.917\times10^{5}T^{-2}$
$H°-H°_{298} = 29.936\times10^{-3}T + 15.568\times10^{-6}T^{2} + 3.917\times10^{2}T^{-1} - 11.623$
880-1800 K: $Cp° = 48.500$
$H°-H°_{298} = 48.500\times10^{-3}T - 15.458$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -261.729 + 12.922\times10^{-3}T - 1.860\times10^{-6}T^{2} + 817.300T^{-1}$
$\Delta Gf° = -261.729 - 12.922\times10^{-3}T\ln T + 1.860\times10^{-6}T^{2} + 408.650T^{-1} + 177.522\times10^{-3}T$
631-750 K: $\Delta Hf° = -259.180 + 4.598\times10^{-3}T + 5.165\times10^{-6}T^{2} + 758.300T^{-1}$
$\Delta Gf° = -259.180 - 4.598\times10^{-3}T\ln T - 5.165\times10^{-6}T^{2} + 379.150T^{-1} + 124.322\times10^{-3}T$
750-880 K: $\Delta Hf° = -262.090 + 10.847\times10^{-3}T + 1.263\times10^{-6}T^{2} + 1071.900T^{-1}$
$\Delta Gf° = -262.090 - 10.847\times10^{-3}T\ln T - 1.263\times10^{-6}T^{2} + 535.950T^{-1} + 166.366\times10^{-3}T$
880-1043 K: $\Delta Hf° = -265.925 + 29.411\times10^{-3}T - 14.305\times10^{-6}T^{2} + 680.200T^{-1}$
$\Delta Gf° = -265.925 - 29.411\times10^{-3}T\ln T + 14.305\times10^{-6}T^{2} + 340.100T^{-1} + 283.140\times10^{-3}T$
1043-1185 K: $\Delta Hf° = -218.803 - 58.551\times10^{-3}T + 27.117\times10^{-6}T^{2} + 223.200T^{-1}$
$\Delta Gf° = -218.803 + 58.551\times10^{-3}T\ln T - 27.117\times10^{-6}T^{2} + 111.600T^{-1} - 329.949\times10^{-3}T$
1185-1667 K: $\Delta Hf° = -266.031 + 17.959\times10^{-3}T - 4.265\times10^{-6}T^{2} + 461.200T^{-1}$
$\Delta Gf° = -266.031 - 17.959\times10^{-3}T\ln T + 4.265\times10^{-6}T^{2} + 230.600T^{-1} + 214.133\times10^{-3}T$
1667-1728 K: $\Delta Hf° = -431.821 + 114.953\times10^{-3}T - 23.527\times10^{-6}T^{2} + 95859.600T^{-1}$
$\Delta Gf° = -431.821 - 114.953\times10^{-3}T\ln T + 23.527\times10^{-6}T^{2} + 47929.800T^{-1} + 983.889\times10^{-3}T$
1728-1800 K: $\Delta Hf° = -431.887 + 110.724\times10^{-3}T - 22.370\times10^{-6}T^{2} + 95546.000T^{-1}$
$\Delta Gf° = -431.887 - 110.724\times10^{-3}T\ln T + 22.370\times10^{-6}T^{2} + 47773.000T^{-1} + 954.453\times10^{-3}T$

Source: Data from Mah (320) who estimated zero point entropy.

NiH(g)
Nickel Hydride (ideal gas)
[Formation: $Ni(c,l) + 0.5H_2(g) = NiH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	6.985	50.319	50.319	0	94.000	85.778	-62.876
300	6.986	50.362	50.319	.013	93.994	85.727	-62.452
400	7.071	52.381	50.594	.715	93.697	83.014	-45.356
500	7.230	53.975	51.115	1.430	93.353	80.382	-35.134
600	7.429	55.310	51.707	2.162	92.953	77.822	-28.346
631	7.493	55.686	51.893	2.393	92.807	77.045	-26.685
700	7.635	56.471	52.305	2.916	92.558	75.339	-23.521
800	7.829	57.503	52.892	3.689	92.241	72.897	-19.914
900	8.002	58.436	53.457	4.481	91.930	70.497	-17.119
1000	8.154	59.287	53.998	5.289	91.617	68.130	-14.889
1100	8.286	60.070	54.515	6.111	91.298	65.806	-13.074
1200	8.399	60.796	55.009	6.945	90.967	63.500	-11.565
1300	8.498	61.473	55.481	7.790	90.625	61.221	-10.292
1400	8.584	62.106	55.932	8.644	90.265	58.974	-9.206
1500	8.660	62.701	56.363	9.507	89.888	56.751	-8.268
1600	8.727	63.262	56.777	10.376	89.489	54.557	-7.452
1700	8.786	63.792	57.173	11.252	89.069	52.378	-6.734
1728	8.801	63.936	57.282	11.498	88.947	51.790	-6.550
1728	8.801	63.936	57.282	11.498	84.847	51.790	-6.550
1800	8.840	64.296	57.555	12.133	84.525	50.415	-6.121
1900	8.888	64.775	57.922	13.020	84.079	48.529	-5.582
2000	8.933	65.233	58.278	13.911	83.632	46.673	-5.100

Phase changes: 631 K, Curie temperature of Ni; $\Delta H^\circ = 0$ kcal/mol.
1728 K, melting point of Ni; $\Delta H^\circ = 4.100$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 6.720 + 1.316\times10^{-3}T - 0.113\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 6.720\times10^{-3}T + 0.658\times10^{-6}T^{2} + 0.113\times10^{2}T^{-1} - 2.100$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = 93.929 + 0.496\times10^{-3}T - 3.832\times10^{-6}T^{2} + 78.550T^{-1}$
$\Delta Gf^\circ = 93.929 - 0.496\times10^{-3}T\ln T + 3.832\times10^{-6}T^{2} + 39.275T^{-1} - 26.096\times10^{-3}T$
631-750 K: $\Delta Hf^\circ = 96.478 - 7.828\times10^{-3}T + 3.193\times10^{-6}T^{2} + 19.550T^{-1}$
$\Delta Gf^\circ = 96.478 + 7.828\times10^{-3}T\ln T - 3.193\times10^{-6}T^{2} + 9.775T^{-1} - 79.296\times10^{-3}T$
750-1728 K: $\Delta Hf^\circ = 93.568 - 1.579\times10^{-3}T - 0.709\times10^{-6}T^{2} + 333.150T^{-1}$
$\Delta Gf^\circ = 93.568 + 1.579\times10^{-3}T\ln T + 0.709\times10^{-6}T^{2} + 166.575T^{-1} - 37.253\times10^{-3}T$
1728-2000 K: $\Delta Hf^\circ = 93.503 - 5.808\times10^{-3}T + 0.448\times10^{-6}T^{2} + 19.550T^{-1}$
$\Delta Gf^\circ = 93.503 + 5.808\times10^{-3}T\ln T - 0.448\times10^{-6}T^{2} + 9.775T^{-1} - 66.689\times10^{-3}T$

Source: Data from Mah (320).

$Ni_2Mg(c)$
Dinickel Magnesium
[Formation: $2Ni(c) + Mg(c) = Ni_2Mg(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.553	21.204	21.204	0	-13.200	-12.936	9.482
300	17.576	21.313	21.206	.032	-13.203	-12.934	9.422
350	18.149	24.067	21.421	.926	-13.248	-12.888	8.047
400	18.580	26.520	21.908	1.845	-13.304	-12.832	7.011
450	18.906	28.728	22.546	2.782	-13.377	-12.773	6.203
467	19.003	29.431	22.782	3.105	-13.406	-12.749	5.966
500	19.186	30.735	23.265	3.735	-13.473	-12.700	5.551
550	19.454	32.576	24.029	4.701	-13.590	-12.618	5.014

Phase change: 467 K, second order transition point of Ni_2Mg; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-467 K: $Cp° = 17.527 + 4.400x10^{-3}T - 1.142x10^{5}T^{-2}$
$H°- H^\circ_{298} = 17.527x10^{-3}T + 2.200x10^{-6}T^{2} + 1.142x10^{2}T^{-1} - 5.804$
467-550 K: $Cp° = 16.422 + 5.520x10^{-3}T$
$H°- H^\circ_{298} = 16.422x10^{-3}T + 2.760x10^{-6}T^{2} - 5.166$

Formation equations (kcal/mol):

298.15-467 K: $\Delta Hf° = -15.189 + 6.392x10^{-3}T - 7.748x10^{-6}T^{2} + 230.300T^{-1}$
$\Delta Gf° = -15.189 - 6.392x10^{-3}TlnT + 7.748x10^{-6}T^{2} + 115.150T^{-1} + 40.372x10^{-3}T$
467-550 K: $\Delta Hf° = -14.551 + 5.287x10^{-3}T - 7.188x10^{-6}T^{2} + 116.100T^{-1}$
$\Delta Gf° = -14.551 - 5.287x10^{-3}TlnT + 7.188x10^{-6}T^{2} + 58.050T^{-1} + 32.737x10^{-3}T$

Source: Data from Mah (320).

$Ni(NH_3)_2I_2(c)$
Diammine Nickel Diiodide
[Formation: $Ni(c) + N_2(g) + 3H_2(g) + I_2(c,l,g) = Ni(NH_3)_2I_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	36.230	59.080	59.080	0	-80.100	-45.750	33.536
300	36.330	59.300	59.080	.070	-80.118	-45.533	33.171
350	38.310	65.060	59.546	1.930	-80.630	-39.738	24.813
386.8	39.561	68.955	60.256	3.365	-81.005	-35.418	20.012
386.8	39.561	68.955	60.256	3.365	-84.714	-35.418	20.012
400	40.010	70.290	60.565	3.890	-84.901	-33.733	18.430
450	41.350	75.070	61.892	5.930	-85.570	-27.285	13.251
458.4	41.498	75.836	62.141	6.278	-85.679	-26.196	12.489
458.4	41.498	75.836	62.141	6.278	-95.700	-26.196	12.489
500	42.230	79.490	63.450	8.020	-95.799	-19.890	8.694
550	42.590	83.530	65.094	10.140	-95.908	-12.297	4.886

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 39.952 + 8.868\times10^{-3}T - 5.659\times10^{5}T^{-2}$
$H° - H°_{298} = 39.952\times10^{-3}T + 4.434\times10^{-6}T^{2} + 5.659\times10^{2}T^{-1} - 14.204$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -81.567 - 1.806\times10^{-3}T - 3.184\times10^{-6}T^{2} + 682.300T^{-1}$
$\Delta Gf° = -81.567 + 1.806\times10^{-3}T\ln T + 3.184\times10^{-6}T^{2} + 341.150T^{-1} + 105.052\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -83.022 - 8.210\times10^{-3}T - 1.692\times10^{-6}T^{2} + 682.300T^{-1}$
$\Delta Gf° = -83.022 + 8.210\times10^{-3}T\ln T + 1.692\times10^{-6}T^{2} + 341.150T^{-1} + 71.237\times10^{-3}T$
458.4-550 K: $\Delta Hf° = -97.735 + 2.130\times10^{-3}T - 1.760\times10^{-6}T^{2} + 667.000T^{-1}$
$\Delta Gf° = -97.735 - 2.130\times10^{-3}T\ln T + 1.760\times10^{-6}T^{2} + 333.500T^{-1} + 166.700\times10^{-3}T$

Source: Data based on Worswick (535).

$Ni(NH_3)_6I_2(c)$
Hexammine Nickel Diiodide
[Formation: $Ni(c) + 3N_2(g) + 9H_2(g) + I_2(c,l,g) = Ni(NH_3)_6I_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	73.470	108.080	108.080	0	-190.900	-88.041	64.535
300	73.680	108.530	108.080	.140	-190.952	-87.399	63.669
350	79.250	120.310	108.996	3.960	-192.277	-70.034	43.731
386.8	83.195	128.424	110.450	6.952	-193.142	-57.131	32.280
386.8	83.195	128.424	110.450	6.952	-196.851	-57.131	32.280
400	84.610	131.240	111.090	8.060	-197.193	-52.357	28.606
450	89.820	141.510	113.910	12.420	-198.340	-34.186	16.603
458.4	90.655	143.179	114.431	13.178	-198.510	-31.121	14.837
458.4	90.655	143.179	114.431	13.178	-208.531	-31.121	14.837
500	94.790	151.240	117.160	17.040	-208.841	-15.003	6.558
550	99.430	160.490	120.690	21.890	-209.028	4.382	-1.741

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 48.890 + 94.122\times10^{-3}T - 3.095\times10^{5}T^{-2}$
$H° - H°_{298} = 48.890\times10^{-3}T + 47.061\times10^{-6}T^{2} + 3.095\times10^{2}T^{-1} - 19.798$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -182.583 - 44.638\times10^{-3}T + 35.751\times10^{-6}T^{2} + 540.700T^{-1}$
$\Delta Gf° = -182.583 + 44.638\times10^{-3}T\ln T - 35.751\times10^{-6}T^{2} + 270.350T^{-1} + 70.383\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -184.038 - 51.042\times10^{-3}T + 37.243\times10^{-6}T^{2} + 540.700T^{-1}$
$\Delta Gf° = -184.038 + 51.042\times10^{-3}T\ln T - 37.243\times10^{-6}T^{2} + 270.350T^{-1} + 36.568\times10^{-3}T$
458.4-550 K: $\Delta Hf° = -198.751 - 40.702\times10^{-3}T + 37.175\times10^{-6}T^{2} + 525.400T^{-1}$
$\Delta Gf° = -198.751 + 40.702\times10^{-3}T\ln T - 37.175\times10^{-6}T^{2} + 262.700T^{-1} + 132.031\times10^{-3}T$

Source: Data based on Worswick (535).

$Ni(OH)_2(g)$
Nickel Dihydroxide (ideal gas)
[Formation: $Ni(c,l) + O_2(g) + H_2(g) = Ni(OH)_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	14.250	69.571	69.571	0	-61.000	-55.699	40.828
300	14.294	69.659	69.572	.026	-61.012	-55.666	40.552
400	16.396	74.071	70.159	1.565	-61.529	-53.803	29.396
500	18.021	77.912	71.332	3.290	-61.944	-51.821	22.651
600	19.247	81.311	72.718	5.156	-62.315	-49.764	18.126
631	19.536	82.288	73.164	5.757	-62.439	-49.111	17.010
700	20.180	84.352	74.168	7.129	-62.620	-47.641	14.874
800	20.906	87.096	75.615	9.185	-62.805	-45.492	12.428
900	21.489	89.593	77.031	11.306	-62.957	-43.319	10.519
1000	21.969	91.882	78.403	13.479	-63.091	-41.133	8.989
1100	22.374	93.996	79.726	15.697	-63.216	-38.921	7.733
1200	22.721	95.958	80.998	17.952	-63.341	-36.709	6.686
1300	23.021	97.789	82.220	20.240	-63.470	-34.488	5.798
1400	23.283	99.505	83.394	22.555	-63.610	-32.253	5.035
1500	23.514	101.119	84.522	24.895	-63.764	-30.010	4.372
1600	23.717	102.643	85.607	27.257	-63.936	-27.750	3.790
1700	23.897	104.086	86.652	29.638	-64.126	-25.492	3.277
1728	23.942	104.477	86.938	30.308	-64.184	-24.840	3.142
1728	23.942	104.477	86.938	30.308	-68.284	-24.840	3.142
1800	24.056	105.457	87.659	32.036	-68.440	-23.030	2.796
1900	24.199	106.761	88.630	34.449	-68.657	-20.505	2.359
2000	24.326	108.006	89.568	36.875	-68.875	-17.961	1.963

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.198 + 3.788\times10^{-3}T - 4.514\times10^{5}T^{-2}$
$H°- H^\circ_{298} = 18.198\times10^{-3}T + 1.894\times10^{-6}T^{2} + 4.514\times10^{2}T^{-1} - 7.108$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -62.774 + 1.516\times10^{-3}T - 3.308\times10^{-6}T^{2} + 481.700T^{-1}$
$\Delta Gf° = -62.774 - 1.516\times10^{-3}T\ln T + 3.308\times10^{-6}T^{2} + 240.850T^{-1} + 28.671\times10^{-3}T$
631-750 K: $\Delta Hf° = -60.225 - 6.808\times10^{-3}T + 3.717\times10^{-6}T^{2} + 422.700T^{-1}$
$\Delta Gf° = -60.225 + 6.808\times10^{-3}T\ln T - 3.717\times10^{-6}T^{2} + 211.350T^{-1} - 24.528\times10^{-3}T$
750-1728 K: $\Delta Hf° = -63.135 - 0.559\times10^{-3}T - 0.185\times10^{-6}T^{2} + 736.300T^{-1}$
$\Delta Gf° = -63.135 + 0.559\times10^{-3}T\ln T + 0.185\times10^{-6}T^{2} + 368.150T^{-1} + 17.515\times10^{-3}T$
1728-2000 K: $\Delta Hf° = -63.200 - 4.788\times10^{-3}T + 0.972\times10^{-6}T^{2} + 422.700T^{-1}$
$\Delta Gf° = -63.200 + 4.788\times10^{-3}T\ln T - 0.972\times10^{-6}T^{2} + 211.350T^{-1} - 11.921\times10^{-3}T$

Source: Data from Mah (320) who estimated molecular constants.

$NiSO_4(c)$
Nickel Sulfate
[Reaction: $Ni(c) + 0.5S_2(g) + 2O_2(g) = NiSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	23.330	24.210	24.210	0	-224.065	-191.807	140.597
300	23.420	24.350	24.217	0.040	-224.070	-191.608	139.585
400	27.510	31.710	25.185	2.610	-223.971	-180.794	98.780
500	30.050	38.140	27.140	5.500	-223.667	-170.028	74.318
600	31.910	43.790	29.457	8.600	-223.283	-159.339	58.039
631	32.363	45.409	30.201	9.596	-223.166	-156.037	54.043
700	33.370	48.820	31.863	11.870	-222.797	-148.707	46.428
800	34.570	53.360	34.285	15.260	-222.176	-138.181	37.749
900	35.560	57.490	36.634	18.770	-221.482	-127.720	31.014
1000	36.380	61.280	38.910	22.370	-220.741	-117.343	25.645
1100	37.030	64.780	41.107	26.040	-219.975	-107.032	21.265
1200	37.530	68.020	43.212	29.770	-219.188	-96.795	17.629

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 28.536 + 8.652\times10^{-3}T - 6.921\times10^{5}T^{-2}$

$H°-H°_{298} = 28.536\times10^{-3}T + 4.326\times10^{-6}T^{2} + 6.921\times10^{2}T^{-1} - 11.214$

Reaction equations (kcal/mol):

298.15-631 K: $\Delta Hr° = -228.127 + 6.908\times10^{-3}T - 1.120\times10^{-6}T^{2} + 626.550T^{-1}$

$\Delta Gr° = -228.127 - 6.908\times10^{-3}T\ln T + 1.120\times10^{-6}T^{2} + 313.275T^{-1} + 157.320\times10^{-3}T$

631-750 K: $\Delta Hr° = -225.578 - 1.416\times10^{-3}T + 5.905\times10^{-6}T^{2} + 567.550T^{-1}$

$\Delta Gr° = -225.578 + 1.416\times10^{-3}T\ln T - 5.905\times10^{-6}T^{2} + 283.775T^{-1} + 104.120\times10^{-3}T$

750-1200 K: $\Delta Hr° = -228.488 + 4.833\times10^{-3}T + 2.003\times10^{-6}T^{2} + 881.150T^{-1}$

$\Delta Gr° = -228.488 - 4.833\times10^{-3}T\ln T - 2.003\times10^{-6}T^{2} + 440.575T^{-1} + 146.163\times10^{-3}T$

Source: Data from DeKock (112).

$NiSO_4 \cdot H_2O(c)$
Nickel Sulfate Monohydrate
[Reaction: $Ni(c) + 0.5S_2(g) + 2.5O_2(g) + H_2(g) = NiSO_4 \cdot H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	32.597	32.700	32.700	0	-299.955	-253.619	185.905
300	32.763	32.902	32.702	.060	-299.960	-253.331	184.549
350	37.260	38.290	33.116	1.811	-299.952	-245.558	153.332
400	41.757	43.559	34.094	3.786	-299.754	-237.799	129.926
450	46.253	48.737	35.433	5.987	-299.360	-230.076	111.739
500	50.750	53.843	37.019	8.412	-298.778	-222.407	97.213
550	55.246	58.891	38.778	11.062	-298.002	-214.808	85.356

*Data except enthalpy of formation and entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 5.631 + 90.204\times10^{-3}T + 0.064\times10^{5}T^{-2}$

$H°-H°_{298} = 5.631\times10^{-3}T + 45.102\times10^{-6}T^{2} - 0.064\times10^{2}T^{-1} - 5.667$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -295.387 - 26.067\times10^{-3}T + 38.985\times10^{-6}T^{2} - 78.050T^{-1}$

$\Delta Gr° = -295.387 + 26.067\times10^{-3}T\ln T - 38.985\times10^{-6}T^{2} - 39.025T^{-1} + 3.631\times10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation and entropy at 298 K.

$NiSO_4 \cdot 4H_2O(c)$

Nickel Sulfate Tetrahydrate

[Reaction: $Ni(c) + 0.5S_2(g) + 4O_2(g) + 4H_2(g) = NiSO_4 \cdot 4H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H^\circ_{298})/T$	$H°-H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	60.500	61.000	61.000	0	-514.755	-427.027	313.015
300	60.767	61.375	61.002	.112	-514.766	-426.482	310.688
350	67.973	71.283	61.766	3.331	-514.858	-411.757	257.109
400	75.180	80.830	63.555	6.910	-514.635	-397.039	216.929
450	82.387	90.102	65.993	10.849	-514.096	-382.370	185.702
500	89.593	99.155	68.859	15.148	-513.240	-367.776	160.753
550	96.800	108.032	72.017	19.808	-512.065	-353.286	140.381

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 17.673 + 143.878 \times 10^{-3}T - 0.062 \times 10^{5}T^{-2}$

$H°-H^\circ_{298} = 17.673 \times 10^{-3}T + 71.939 \times 10^{-6}T^{2} + 0.062 \times 10^{2}T^{-1} - 11.685$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -506.957 - 44.238 \times 10^{-3}T + 63.811 \times 10^{-6}T^{2} - 83.750T^{-1}$

$\Delta Gr° = -506.957 + 44.238 \times 10^{-3}T\ln T - 63.811 \times 10^{-6}T^{2} - 41.875T^{-1} + 35.529 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$NiSO_4 \cdot 6H_2O(\alpha)$
α-Nickel Sulfate Hexahydrate
[Reaction: $Ni(c) + 0.5S_2(g) + 5O_2(g) + 6H_2(g) = NiSO_4 \cdot 6H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	78.361	79.935	79.935	0	-656.695	-541.393	396.847
300*	78.730	80.421	79.938	.145	-656.712	-540.678	393.878
350	88.180	93.280	80.931	4.322	-656.891	-521.319	325.522
400	96.579	105.615	83.250	8.946	-656.676	-501.960	274.255
450	103.928	117.425	86.396	13.963	-656.120	-482.652	234.405
500	110.227	128.710	90.068	19.321	-655.274	-463.420	202.558
550	115.476	139.470	94.074	24.968	-654.185	-444.288	176.542

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 65.315 + 101.930\text{x}10^{-3}T - 15.418\text{x}10^{5}T^{-2}$

$H° - H°_{298} = 65.315\text{x}10^{-3}T + 50.965\text{x}10^{-6}T^{2} + 15.418\text{x}10^{2}T^{-1} - 29.175$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -660.222 - 16.739\text{x}10^{-3}T + 41.496\text{x}10^{-6}T^{2} + 1439.650T^{-1}$

$\Delta Gr° = -660.222 + 16.739\text{x}10^{-3}T\ln T - 41.496\text{x}10^{-6}T^{2} + 719.825T^{-1} + 307.459\text{x}10^{-3}T$

Source: Data from DeKocK (112) who estimated all above 298 K.

$NiSO_4 \cdot 7H_2O(c)$
Nickel Sulfate Heptahydrate
[Reaction: $Ni(c) + 0.5S_2(g) + 5.5O_2(g) + 7H_2(g) = NiSO_4 \cdot 7H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	87.142	90.570	90.570	0	-726.755	-598.014	438.350
300	87.503	91.110	90.570	.162	-726.775	-597.214	435.065
304	88.277	92.274	90.587	.513	-726.812	-595.487	428.099
350	96.425	105.290	91.670	4.767	-727.048	-575.594	359.413
400	103.728	118.660	94.218	9.777	-726.974	-553.959	302.665
450	109.412	131.222	97.640	15.112	-726.631	-532.352	258.542
500	113.477	142.974	101.592	20.691	-726.097	-510.792	223.264
550	115.923	153.917	105.857	26.433	-725.451	-489.295	194.425

Phase change: 304 K, $NiSO_4 \cdot 7H_2O$ dissociates to $NiSO_4 \cdot 6H_2O$ and saturated solution.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 100.572 + 44.440 \times 10^{-3}T - 23.717 \times 10^{5}T^{-2}$
$H°- H°_{298} = 100.572 \times 10^{-3}T + 22.220 \times 10^{-6}T^{2} + 23.717 \times 10^{2}T^{-1} - 39.915$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -737.939 + 8.447 \times 10^{-3}T + 12.081 \times 10^{-6}T^{2} + 2263.450T^{-1}$
$\Delta Gr° = -737.939 - 8.447 \times 10^{-3}T\ln T - 12.081 \times 10^{-6}T^{2} + 1131.725T^{-1} + 508.312 \times 10^{-3}T$

Source: Data from DeKock (112).

$NiSe_{1.05}(c)$
Nickel Selenide
[Reaction: $Ni(c) + 0.525Se_2(g) = NiSe_{1.05}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	12.640	17.975	17.975	0	-35.382	-29.503	21.626
300	12.650	18.054	17.977	.023	-35.381	-29.467	21.467
400	13.190	21.773	18.483	1.316	-35.262	-27.516	15.034
500	13.640	24.765	19.449	2.658	-35.160	-25.592	11.186
600	14.110	27.294	20.552	4.045	-35.085	-23.691	8.629
631	14.277	28.009	20.901	4.485	-35.079	-23.100	8.001
700	14.650	29.507	21.676	5.482	-34.977	-21.790	6.803
800	15.300	31.506	22.781	6.980	-34.745	-19.923	5.443
900	15.950	33.343	23.853	8.541	-34.459	-18.088	4.392
1000	16.880	35.069	24.891	10.178	-34.108	-16.294	3.561
1050	17.720	35.912	25.388	11.050	-33.884	-15.390	3.203

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1050 K:

$$Cp^\circ = 10.741 + 5.702\times10^{-3}T + 0.177\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 10.741\times10^{-3}T + 2.851\times10^{-6}T^{2} - 0.177\times10^{2}T^{-1} - 3.396$$

Reaction equations (kcal/mol):

298.15-631 K:

$$\Delta Hr^\circ = -35.943 + 2.146\times10^{-3}T - 1.262\times10^{-6}T^{2} + 9.853T^{-1}$$

$$\Delta Gr^\circ = -35.943 - 2.146\times10^{-3}T\ln T + 1.262\times10^{-6}T^{2} + 4.926T^{-1} + 33.399\times10^{-3}T$$

631-750 K:

$$\Delta Hr^\circ = -33.394 - 6.178\times10^{-3}T + 5.763\times10^{-6}T^{2} - 49.147T^{-1}$$

$$\Delta Gr^\circ = -33.394 + 6.178\times10^{-3}T\ln T - 5.763\times10^{-6}T^{2} - 24.574T^{-1} - 19.801\times10^{-3}T$$

750-1050 K:

$$\Delta Hr^\circ = -36.305 + 0.071\times10^{-3}T + 1.861\times10^{-6}T^{2} + 264.452T^{-1}$$

$$\Delta Gr^\circ = -36.305 - 0.071\times10^{-3}T\ln T - 1.861\times10^{-6}T^{2} + 132.226T^{-1} + 22.243\times10^{-3}T$$

Source: Data from Mah (320).

$NiSe_{1.14}(c)$
Nickel Selenide
[Reaction: $Ni(c) + 0.570Se_2(g) = NiSe_{1.14}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°₂₉₈)/T	H°- H°₂₉₈	ΔHr°	ΔGr°	
298.15	13.130	18.446	18.446	0	-37.981	-31.461	23.061
300	13.150	18.527	18.447	.024	-37.979	-31.421	22.890
400	14.030	22.438	18.976	1.385	-37.837	-29.257	15.985
500	21.730	25.811	20.003	2.904	-37.603	-27.133	11.860
503	23.540	25.904	19.940	3.000	-37.547	-27.021	11.740
600	14.950	28.645	21.225	4.452	-37.413	-25.068	9.131
631	15.096	29.402	21.608	4.918	-37.395	-24.429	8.461
700	15.420	30.981	22.452	5.970	-37.269	-23.011	7.184
800	15.980	33.075	23.651	7.539	-37.012	-20.993	5.735
900	16.690	34.994	24.804	9.171	-36.700	-19.008	4.616
1000	17.530	36.796	25.915	10.881	-36.321	-17.068	3.730
1050	17.990	37.663	26.454	11.769	-36.104	-16.100	3.351

Phase changes: 503 K, second order transition point of $NiSe_{1.14}$; ΔH° = 0 kcal/mol.
631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-503 K: $Cp° = -3.215 + 36.504x10^{-3}T + 4.855x10^{5}T^{-2}$
$H°- H°_{298} = -3.215x10^{-3}T + 18.252x10^{-6}T^{2} - 4.855x10^{2}T^{-1} + 0.964$
503-1050 K: $Cp° = 11.945 + 5.206x10^{-3}T$
$H°- H°_{298} = 11.945x10^{-3}T + 2.603x10^{-6}T^{2} - 3.667$

Reaction equations (kcal/mol):

298.15-503 K: $\Delta Hr° = -34.030 - 12.289x10^{-3}T + 14.154x10^{-6}T^{2} - 460.643T^{-1}$
$\Delta Gr° = -34.030 + 12.289x10^{-3}TlnT - 14.154x10^{-6}T^{2} - 230.322T^{-1} - 54.593x10^{-3}T$
503-631 K: $\Delta Hr° = -38.661 + 2.871x10^{-3}T - 1.495x10^{-6}T^{2} + 24.857T^{-1}$
$\Delta Gr° = -38.661 - 2.871x10^{-3}TlnT + 1.495x10^{-6}T^{2} + 12.428T^{-1} + 40.088x10^{-3}T$
631-750 K: $\Delta Hr° = -36.113 - 5.453x10^{-3}T + 5.530x10^{-6}T^{2} - 34.143T^{-1}$
$\Delta Gr° = -36.113 + 5.453x10^{-3}TlnT - 5.530x10^{-6}T^{2} - 17.072T^{-1} - 13.112x10^{-3}T$
750-1050 K: $\Delta Hr° = -39.023 + 0.796x10^{-3}T + 1.628x10^{-6}T^{2} + 279.457T^{-1}$
$\Delta Gr° = -39.023 - 0.796x10^{-3}TlnT - 1.628x10^{-6}T^{2} + 139.729T^{-1} + 28.931x10^{-3}T$

Source: Data from Mah (320).

$NiSe_{1.25}(c)$
Nickel Selenide
[Reaction: $Ni(c) + 0.625Se_2(g) = NiSe_{1.25}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	13.590	19.138	19.138	0	-40.612	-33.344	24.442
300	13.600	19.222	19.139	.025	-40.611	-33.300	24.258
400	14.460	23.266	19.684	1.433	-40.477	-30.883	16.873
500	15.180	26.561	20.739	2.911	-40.339	-28.501	12.458
589	18.880	29.267	21.800	4.398	-40.105	-26.399	9.795
600	16.140	29.583	21.965	4.571	-40.092	-26.159	9.528
631	16.227	30.398	22.359	5.073	-40.056	-25.438	8.810
700	16.420	32.079	23.236	6.190	-39.903	-23.843	7.444
800	16.970	34.306	24.482	7.859	-39.601	-21.570	5.892
900	17.880	36.351	25.688	9.597	-39.238	-19.338	4.696
995	18.930	38.215	26.798	11.360	-38.792	-17.266	3.792
1000	18.760	38.310	26.855	11.455	-38.767	-17.158	3.750
1050	19.130	39.231	27.422	12.399	-38.520	-16.073	3.345

Phase changes: 589 K, second order transition point of $NiSe_{1.25}$; ΔH° = 0 kcal/mol.
631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
995 K, second order transition point of $NiSe_{1.25}$; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-589 K: $Cp° = 2.828 + 23.390 \times 10^{-3}T + 3.367 \times 10^{5}T^{-2}$
$H° - H°_{298} = 2.828 \times 10^{-3}T + 11.695 \times 10^{-6}T^{2} - 3.367 \times 10^{2}T^{-1} - 0.753$
589-995 K: $Cp° = 11.097 + 7.640 \times 10^{-3}T$
$H° - H°_{298} = 11.097 \times 10^{-3}T + 3.820 \times 10^{-6}T^{2} - 3.463$
995-1050 K: $Cp° = 23.353 - 4.364 \times 10^{-3}T$
$H° - H°_{298} = 23.353 \times 10^{-3}T - 2.182 \times 10^{-6}T^{2} - 9.716$

Reaction equations (kcal/mol):

298.15-589 K: $\Delta Hr° = -38.195 - 6.833 \times 10^{-3}T + 7.614 \times 10^{-6}T^{2} - 315.138T^{-1}$
$\Delta Gr° = -38.195 + 6.833 \times 10^{-3}T\ln T - 7.614 \times 10^{-6}T^{2} - 157.569T^{-1} - 18.620 \times 10^{-3}T$
589-631 K: $\Delta Hr° = -40.905 + 1.436 \times 10^{-3}T - 0.261 \times 10^{-6}T^{2} + 21.563T^{-1}$
$\Delta Gr° = -40.905 - 1.436 \times 10^{-3}T\ln T + 0.261 \times 10^{-6}T^{2} + 10.781T^{-1} + 33.601 \times 10^{-3}T$
631-750 K: $\Delta Hr° = -38.356 - 6.888 \times 10^{-3}T + 6.764 \times 10^{-6}T^{2} - 37.438T^{-1}$
$\Delta Gr° = -38.356 + 6.888 \times 10^{-3}T\ln T - 6.764 \times 10^{-6}T^{2} - 18.719T^{-1} - 19.599 \times 10^{-3}T$
750-995 K: $\Delta Hr° = -41.266 - 0.639 \times 10^{-3}T + 2.862 \times 10^{-6}T^{2} + 276.163T^{-1}$
$\Delta Gr° = -41.266 + 0.639 \times 10^{-3}T\ln T - 2.862 \times 10^{-6}T^{2} + 138.081T^{-1} + 22.445 \times 10^{-3}T$
995-1050 K: $\Delta Hr° = -47.519 + 11.617 \times 10^{-3}T - 3.140 \times 10^{-6}T^{2} + 276.163T^{-1}$
$\Delta Gr° = -47.519 - 11.617 \times 10^{-3}T\ln T + 3.140 \times 10^{-6}T^{2} + 138.081T^{-1} + 107.357 \times 10^{-3}T$

Source: Data from Mah (320).

$NiSe_2(c)$
Nickel Diselenide
[Reaction: $Ni(c) + Se_2(g) = NiSe_2(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	18.028	24.740	24.740	0	-53.300	-41.195	30.196
300	18.047	24.852	24.742	.033	-53.297	-41.121	29.956
400	18.929	30.168	25.460	1.883	-53.094	-37.093	20.267
500	19.458	34.451	26.843	3.804	-52.891	-33.117	14.475
600	19.900	38.037	28.417	5.772	-52.716	-29.182	10.629
631	20.018	39.042	28.915	6.391	-52.680	-27.965	9.686
700	20.282	41.135	30.018	7.782	-52.514	-25.267	7.888
800	20.538	43.860	31.581	9.823	-52.218	-21.394	5.844
900	21.006	46.302	33.083	11.897	-51.896	-17.563	4.265
1000	22.077	48.564	34.519	14.045	-51.509	-13.773	3.010

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 18.476 + 2.878x10^{-3}T - 1.161x10^{5}T^{-2}$
$H°- H°_{298} = 18.476x10^{-3}T + 1.439x10^{-6}T^{2} + 1.161x10^{2}T^{-1} - 6.026$

Reaction equations (kcal/mol):

298.15-631 K: $ΔHr° = -54.898 + 4.816x10^{-3}T - 2.522x10^{-6}T^{2} + 115.200T^{-1}$
$ΔGr° = -54.898 - 4.816x10^{-3}TlnT + 2.522x10^{-6}T^{2} + 57.600T^{-1} + 72.000x10^{-3}T$
631-750 K: $ΔHr° = -52.349 - 3.508x10^{-3}T + 4.503x10^{-6}T^{2} + 56.200T^{-1}$
$ΔGr° = -52.349 + 3.508x10^{-3}TlnT - 4.503x10^{-6}T^{2} + 28.100T^{-1} + 18.800x10^{-3}T$
750-1000 K: $ΔHr° = -55.259 + 2.741x10^{-3}T + 0.601x10^{-6}T^{2} + 369.800T^{-1}$
$ΔGr° = -55.259 - 2.741x10^{-3}TlnT - 0.601x10^{-6}T^{2} + 184.900T^{-1} + 60.843x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mah (320). Low-temperature heat capacities and entropy at 298 K from Gronvold (191). High-temperature data from Gronvold (185).

NiSi(c,l)
Nickel Silicide
[Formation: Ni(c) + Si(c) = NiSi(c,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	10.700	11.200	11.200	0	-20.600	-20.469	15.004
300	10.700	11.200	11.200	.020	-20.601	-20.448	14.896
400	11.800	14.500	11.625	1.150	-20.630	-20.418	11.156
500	12.400	17.200	12.460	2.370	-20.666	-20.351	8.895
600	12.800	19.500	13.450	3.630	-20.760	-20.286	7.389
631	12.862	20.146	13.763	4.028	-20.812	-20.258	7.016
700	13.000	21.500	14.471	4.920	-20.859	-20.201	6.307
800	13.200	23.200	15.438	6.210	-20.911	-20.087	5.487
900	13.400	24.800	16.411	7.550	-20.939	-20.003	4.857
1000	13.500	26.200	17.310	8.890	-20.989	-19.879	4.344
1100	13.700	27.500	18.182	10.250	-21.044	-19.768	3.927
1200	13.800	28.700	19.000	11.640	-21.094	-19.642	3.577
1265	13.900	29.400	19.495	12.520	-21.163	-19.536	3.375
1265	19.100	37.700	19.495	23.040	-10.643	-19.536	3.375
1300	19.100	38.200	19.962	23.710	-10.489	-19.745	3.319
1400	19.100	39.700	21.400	25.620	-10.071	-20.585	3.213
1500	19.100	41.000	22.647	27.530	-9.681	-21.336	3.109

Phase changes: 631 K, Curie temperature of Ni; $\Delta H^\circ = 0$ kcal/mol.
1265 K, melting point of NiSi; $\Delta H^\circ = 10.520$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1265 K: $Cp^\circ = 12.804 + 0.902\times10^{-3}T - 2.112\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 12.804\times10^{-3}T + 0.451\times10^{-6}T^{2} + 2.112\times10^{2}T^{-1} - 4.566$
1265-1500 K: $Cp^\circ = 19.100$
$H^\circ - H^\circ_{298} = 19.100\times10^{-3}T - 1.122$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -22.035 + 4.129\times10^{-3}T - 4.180\times10^{-6}T^{2} + 171.700T^{-1}$
$\Delta Gf^\circ = -22.035 - 4.129\times10^{-3}T\ln T + 4.180\times10^{-6}T^{2} + 85.850T^{-1} + 26.568\times10^{-3}T$
631-750 K: $\Delta Hf^\circ = -19.487 - 4.195\times10^{-3}T + 2.845\times10^{-6}T^{2} + 112.700T^{-1}$
$\Delta Gf^\circ = -19.487 + 4.195\times10^{-3}T\ln T - 2.845\times10^{-6}T^{2} + 56.350T^{-1} - 26.632\times10^{-3}T$
750-1265 K: $\Delta Hf^\circ = -22.397 + 2.054\times10^{-3}T - 1.057\times10^{-6}T^{2} + 426.300T^{-1}$
$\Delta Gf^\circ = -22.397 - 2.054\times10^{-3}T\ln T + 1.057\times10^{-6}T^{2} + 213.150T^{-1} + 15.411\times10^{-3}T$
1265-1500 K: $\Delta Hf^\circ = -18.952 + 8.350\times10^{-3}T - 1.508\times10^{-6}T^{2} + 215.100T^{-1}$
$\Delta Gf^\circ = -18.952 - 8.350\times10^{-3}T\ln T + 1.508\times10^{-6}T^{2} + 107.550T^{-1} + 57.155\times10^{-3}T$

Source: Data from Mah (320).

$Ni_{1.04}Si_{1.93}(c)$

Nickel Disilicide

[Formation: $1.04Ni(c) + 1.93Si(c) = Ni_{1.04}Si_{1.93}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.649	15.617	15.617	0	-21.400	-21.253	15.579
300	15.688	15.714	15.617	.029	-21.401	-21.252	15.482
400	17.240	20.483	16.258	1.690	-21.396	-21.208	11.588
500	17.946	24.413	17.507	3.453	-21.426	-21.157	9.247
600	18.442	27.730	18.942	5.273	-21.523	-21.100	7.685
631	18.584	28.663	19.397	5.847	-21.579	-21.075	7.299
700	18.899	30.607	20.407	7.140	-21.626	-21.015	6.561
800	19.365	33.161	21.845	9.053	-21.648	-20.925	5.716
900	19.844	35.469	23.232	11.013	-21.662	-20.835	5.059
1000	20.321	37.585	24.563	13.022	-21.658	-20.730	4.530
1100	20.770	39.543	25.837	15.077	-21.641	-20.643	4.101
1200	21.160	41.367	27.055	17.174	-21.615	-20.556	3.744
1245	21.308	42.149	27.588	18.129	-21.602	-20.518	3.602

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1245 K, incongruent melting point of $Ni_{1.04}Si_{1.93}$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1245 K: $Cp° = 17.200 + 3.302\times10^{-3}T - 2.254\times10^{5}T^{-2}$
$H°- H°_{298} = 17.200\times10^{-3}T + 1.651\times10^{-6}T^{2} + 2.254\times10^{2}T^{-1} - 6.031$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -22.346 + 3.124\times10^{-3}T - 3.478\times10^{-6}T^{2} + 96.655T^{-1}$
$\Delta Gf° = -22.346 - 3.124\times10^{-3}T\ln T + 3.478\times10^{-6}T^{2} + 48.327T^{-1} + 19.885\times10^{-3}T$
631-750 K: $\Delta Hf° = -19.696 - 5.533\times10^{-3}T + 3.828\times10^{-6}T^{2} + 35.295T^{-1}$
$\Delta Gf° = -19.696 + 5.533\times10^{-3}T\ln T - 3.828\times10^{-6}T^{2} + 17.647T^{-1} - 35.443\times10^{-3}T$
750-1245 K: $\Delta Hf° = -22.722 + 0.966\times10^{-3}T - 0.230\times10^{-6}T^{2} + 361.439T^{-1}$
$\Delta Gf° = -22.722 - 0.966\times10^{-3}T\ln T + 0.230\times10^{-6}T^{2} + 180.720T^{-1} + 8.282\times10^{-3}T$

Source: Data from Mah (320).

$Ni_2Si(c,l)$
Dinickel Silicide
[Formation: $2Ni(c,l) + Si(c,l) = Ni_2Si(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	16.974	18.300	18.300	0	-33.600	-33.457	24.524
300	17.013	18.405	18.302	.031	-33.602	-33.457	24.373
400	17.954	23.468	18.986	1.793	-33.651	-33.406	18.252
500	18.156	27.498	20.298	3.600	-33.810	-33.329	14.568
600	18.412	30.828	21.783	5.427	-34.119	-33.212	12.097
631	18.552	31.759	22.250	6.000	-34.265	-33.158	11.484
700	18.865	33.698	23.285	7.289	-34.444	-33.022	10.310
800	19.497	36.256	24.749	9.206	-34.606	-32.811	8.963
900	20.259	38.596	26.159	11.193	-34.735	-32.580	7.912
1000	21.114	40.774	27.513	13.261	-34.819	-32.333	7.066
1100	22.061	42.830	28.813	15.419	-34.854	-32.071	6.372
1200	23.134	44.794	30.063	17.677	-34.832	-31.825	5.796
1300	24.413	46.695	31.270	20.052	-34.737	-31.584	5.310
1400	26.024	48.560	32.438	22.571	-34.545	-31.339	4.892
1490	27.898	50.237	33.463	24.993	-34.260	-31.157	4.570
1490	26.200	51.434	33.463	26.777	-32.476	-31.157	4.570
1500	26.200	51.609	33.583	27.039	-32.454	-31.148	4.538
1560	26.200	52.637	34.296	28.611	-32.333	-31.093	4.356
1560	27.700	59.430	34.296	39.209	-21.735	-31.093	4.356
1600	27.700	60.132	34.934	40.317	-21.604	-31.335	4.280
1687	27.700	61.598	36.271	42.727	-21.347	-31.873	4.129
1687	27.700	61.598	36.271	42.727	-33.429	-31.873	4.129
1700	27.700	61.811	36.466	43.087	-33.385	-31.857	4.095
1728	27.700	62.264	36.880	43.863	-33.294	-31.802	4.022
1728	27.700	62.264	36.880	43.863	-41.494	-31.802	4.022
1800	27.700	63.394	37.918	45.857	-41.279	-31.404	3.813

*Entropy at 298 K estimated.

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1490 K, α - β transition point of Ni_2Si; ΔH° = 1.784 kcal/mol.
1560 K, melting point of Ni_2Si; ΔH° = 10.598 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1490 K: $Cp^\circ = 12.890 + 8.704\text{x}10^{-3}T + 1.323\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 12.890\text{x}10^{-3}T + 4.352\text{x}10^{-6}T^2 - 1.323\text{x}10^{2}T^{-1} - 3.786$
1490-1560 K: $Cp^\circ = 26.200$
$H^\circ - H^\circ_{298} = 26.200\text{x}10^{-3}T - 12.261$
1560-1800 K: $Cp^\circ = 27.700$
$H^\circ - H^\circ_{298} = 27.700\text{x}10^{-3}T - 4.003$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -33.180 + 1.219\text{x}10^{-3}T - 4.559\text{x}10^{-6}T^2 - 112.800T^{-1}$
$\Delta Gf^\circ = -33.180 - 1.219\text{x}10^{-3}T\ln T + 4.559\text{x}10^{-6}T^2 - 56.400T^{-1} + 5.291\text{x}10^{-3}T$
631-750 K: $\Delta Hf^\circ = -28.082 - 15.429\text{x}10^{-3}T + 9.491\text{x}10^{-6}T^2 - 230.800T^{-1}$
$\Delta Gf^\circ = -28.082 + 15.429\text{x}10^{-3}T\ln T - 9.491\text{x}10^{-6}T^2 - 115.400T^{-1} - 101.108\text{x}10^{-3}T$
750-1490 K: $\Delta Hf^\circ = -33.902 - 2.931\text{x}10^{-3}T + 1.687\text{x}10^{-6}T^2 + 396.400T^{-1}$
$\Delta Gf^\circ = -33.902 + 2.931\text{x}10^{-3}T\ln T - 1.687\text{x}10^{-6}T^2 + 198.200T^{-1} - 17.021\text{x}10^{-3}T$
1490-1560 K: $\Delta Hf^\circ = -42.377 + 10.379\text{x}10^{-3}T - 2.665\text{x}10^{-6}T^2 + 528.700T^{-1}$
$\Delta Gf^\circ = -42.377 - 10.379\text{x}10^{-3}T\ln T + 2.665\text{x}10^{-6}T^2 + 264.350T^{-1} + 79.402\text{x}10^{-3}T$
1560-1687 K: $\Delta Hf^\circ = -34.119 + 11.879\text{x}10^{-3}T - 2.665\text{x}10^{-6}T^2 + 528.700T^{-1}$
$\Delta Gf^\circ = -34.119 - 11.879\text{x}10^{-3}T\ln T + 2.665\text{x}10^{-6}T^2 + 264.350T^{-1} + 85.137\text{x}10^{-3}T$
1687-1728 K: $\Delta Hf^\circ = -46.548 + 11.458\text{x}10^{-3}T - 2.314\text{x}10^{-6}T^2 + 627.200T^{-1}$
$\Delta Gf^\circ = -46.548 - 11.458\text{x}10^{-3}T\ln T + 2.314\text{x}10^{-6}T^2 + 313.600T^{-1} + 89.951\text{x}10^{-3}T$
1728-1800 K: $\Delta Hf^\circ = -46.679 + 3.000\text{x}10^{-3}T$
$\Delta Gf^\circ = -46.679 - 3.000\text{x}10^{-3}T\ln T + 31.079\text{x}10^{-3}T$

Source: Data from Mah (320) who estimated entropy at 298 K.

$Ni_2SiO_4(c)$
Nickel Silicate
[Formation: $2Ni(c,l) + Si(c,l) + 2O_2(g) = Ni_2SiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	30.467	25.600	25.600	0	-336.000	-308.812	226.362
300	30.572	25.789	25.602	.056	-336.003	-308.643	224.844
400	36.216	35.371	26.868	3.401	-335.889	-299.533	163.655
500	40.563	43.950	29.442	7.254	-335.464	-290.488	126.971
600	43.333	51.612	32.512	11.460	-334.904	-281.551	102.554
631	43.815	53.807	33.505	12.811	-334.750	-278.795	96.561
700	44.888	58.422	35.736	15.880	-334.227	-272.697	85.139
800	45.669	64.473	38.958	20.412	-333.370	-263.972	72.113
900	46.058	69.876	42.097	25.001	-332.525	-255.348	62.006
1000	46.346	74.744	45.123	29.621	-331.711	-246.815	53.941
1100	46.730	79.178	48.021	34.273	-330.930	-238.352	47.356
1200	47.330	83.268	50.790	38.974	-330.161	-229.975	41.884
1300	48.203	87.089	53.437	43.748	-329.379	-221.665	37.265
1400	49.364	90.702	55.971	48.624	-328.558	-213.402	33.313
1500	50.806	94.155	58.402	53.630	-327.669	-205.223	29.901
1600	52.522	97.487	60.741	58.794	-326.687	-197.085	26.920
1687	54.265	100.312	62.709	63.437	-325.731	-190.064	24.622
1687	54.265	100.312	62.709	63.437	-337.813	-190.064	24.622
1700	54.526	100.730	62.998	64.144	-337.652	-188.922	24.287
1728	55.183	101.626	63.617	65.680	-337.297	-186.445	23.580
1728	55.183	101.626	63.617	65.680	-345.497	-186.445	23.580
1800	56.873	103.911	65.183	69.711	-344.525	-179.838	21.835

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp^\circ = 41.760 + 6.314\times10^{-3}T - 11.712\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 41.760\times10^{-3}T + 3.157\times10^{-6}T^{2} + 11.712\times10^{2}T^{-1} - 16.660$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -343.749 + 15.629\times10^{-3}T - 6.760\times10^{-6}T^{2} + 1100.300T^{-1}$
$\Delta Gf^\circ = -343.749 - 15.629\times10^{-3}T\ln T + 6.760\times10^{-6}T^{2} + 550.150T^{-1} + 198.025\times10^{-3}T$
631-750 K: $\Delta Hf^\circ = -338.652 - 1.019\times10^{-3}T + 7.290\times10^{-6}T^{2} + 982.300T^{-1}$
$\Delta Gf^\circ = -338.652 + 1.019\times10^{-3}T\ln T - 7.290\times10^{-6}T^{2} + 491.150T^{-1} + 91.625\times10^{-3}T$
750-1687 K: $\Delta Hf^\circ = -344.472 + 11.479\times10^{-3}T - 0.514\times10^{-6}T^{2} + 1609.500T^{-1}$
$\Delta Gf^\circ = -344.472 - 11.479\times10^{-3}T\ln T + 0.514\times10^{-6}T^{2} + 804.750T^{-1} + 175.712\times10^{-3}T$
1687-1728 K: $\Delta Hf^\circ = -356.901 + 11.058\times10^{-3}T - 0.163\times10^{-6}T^{2} + 1708.000T^{-1}$
$\Delta Gf^\circ = -356.901 - 11.058\times10^{-3}T\ln T + 0.163\times10^{-6}T^{2} + 854.000T^{-1} + 180.526\times10^{-3}T$
1728-1800 K: $\Delta Hf^\circ = -357.032 + 2.600\times10^{-3}T + 2.151\times10^{-6}T^{2} + 1080.800T^{-1}$
$\Delta Gf^\circ = -357.032 - 2.600\times10^{-3}T\ln T - 2.151\times10^{-6}T^{2} + 540.400T^{-1} + 121.654\times10^{-3}T$

Source: Data from Mah (320).

$NiTe_{1.10}(c)$

Nickel Telluride

[Reaction: $Ni(c) + 0.55Te_2(g) = NiTe_{1.10}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	13.090	20.090	20.090	0	-34.782	-28.497	20.889
300	13.110	20.170	20.090	.024	-34.778	-28.459	20.732
400	13.750	24.050	20.620	1.372	-34.566	-26.387	14.417
500	14.130	27.160	21.626	2.767	-34.374	-24.365	10.650
600	14.420	29.760	22.768	4.195	-34.230	-22.376	8.150
631	14.494	30.488	23.130	4.643	-34.208	-21.762	7.537
700	14.660	32.000	23.929	5.650	-34.084	-20.404	6.370
800	14.880	33.970	25.063	7.126	-33.865	-18.469	5.045
900	15.080	35.740	26.158	8.624	-33.644	-16.564	4.022
1000	15.270	37.340	27.198	10.142	-33.425	-14.682	3.209

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 13.740 + 1.608x10^{-3}T - 1.004x10^{5}T^{-2}$

$H°- H°_{298} = 13.740x10^{-3}T + 0.804x10^{-6}T^{2} + 1.004x10^{2}T^{-1} - 4.505$

Reaction equations (kcal/mol):

298.15-631 K: $ΔHr° = -36.727 + 6.015x10^{-3}T - 3.802x10^{-6}T^{2} + 146.090T^{-1}$

$ΔGr° = -36.727 - 6.015x10^{-3}TlnT + 3.802x10^{-6}T^{2} + 73.045T^{-1} + 59.916x10^{-3}T$

631-750 K: $ΔHr° = -34.178 - 2.309x10^{-3}T + 3.223x10^{-6}T^{2} + 87.090T^{-1}$

$ΔGr° = -34.178 + 2.309x10^{-3}TlnT - 3.223x10^{-6}T^{2} + 43.545T^{-1} + 6.716x10^{-3}T$

750-1000 K: $ΔHr° = -37.088 + 3.940x10^{-3}T - 0.679x10^{-6}T^{2} + 400.690T^{-1}$

$ΔGr° = -37.088 - 3.940x10^{-3}TlnT + 0.679x10^{-6}T^{2} + 200.345T^{-1} + 48.760x10^{-3}T$

Source: Data from Mills (332).

$Ni_3Te_4(c)$
Trinickel Tetratelluride
[Reaction: $3Ni(c) + 2Te_2(g) = Ni_3Te_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	42.749	69.601	69.601	0	-123.860	-101.332	74.277
300	42.805	69.866	69.603	.079	-123.849	-101.195	73.719
400	45.906	82.628	71.323	4.522	-123.120	-93.751	51.223
500	46.725	92.974	74.648	9.163	-122.401	-86.493	37.806
600	47.733	101.570	78.435	13.881	-121.855	-79.363	28.908
631	48.323	103.989	79.632	15.370	-121.746	-77.165	26.726
700	49.637	109.067	82.297	18.739	-121.249	-72.317	22.578
800	52.514	115.878	86.076	23.842	-120.249	-65.407	17.868
900	56.000	122.248	89.737	29.260	-118.997	-58.623	14.235
950	57.820	125.328	91.529	32.109	-118.259	-55.297	12.721

*Entropy at 298 K estimated.

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-950 K: $Cp^\circ = 39.855 + 15.596 \times 10^{-3}T - 1.561 \times 10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 39.855 \times 10^{-3}T + 7.798 \times 10^{-6}T^{2} + 1.561 \times 10^{2}T^{-1} - 13.100$

Reaction equations (kcal/mol):

298.15-631 K: $\Delta Hr^\circ = -128.337 + 13.669 \times 10^{-3}T - 6.228 \times 10^{-6}T^{2} + 284.700T^{-1}$
$\Delta Gr^\circ = -128.337 - 13.669 \times 10^{-3}T\ln T + 6.228 \times 10^{-6}T^{2} + 142.350T^{-1} + 164.996 \times 10^{-3}T$
631-750 K: $\Delta Hr^\circ = -120.690 - 11.303 \times 10^{-3}T + 14.847 \times 10^{-6}T^{2} + 107.700T^{-1}$
$\Delta Gr^\circ = -120.690 + 11.303 \times 10^{-3}T\ln T - 14.847 \times 10^{-6}T^{2} + 53.850T^{-1} + 5.396 \times 10^{-3}T$
750-950 K: $\Delta Hr^\circ = -129.420 + 7.444 \times 10^{-3}T + 3.141 \times 10^{-6}T^{2} + 1048.500T^{-1}$
$\Delta Gr^\circ = -129.420 - 7.444 \times 10^{-3}T\ln T - 3.141 \times 10^{-6}T^{2} + 524.250T^{-1} + 131.527 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Soboleva (468). Other data from Gronvold (184) who estimated entropy at 298 K.

$NiTiO_3(c)$
Nickel Titanate
[Formation: $Ni(c) + Ti(c) + 1.5O_2(g) = NiTiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	22.080	20.000	20.000	0	-285.800	-265.535	194.640
300	22.120	20.140	20.007	.040	-285.802	-265.410	193.349
400	23.980	26.780	20.905	2.350	-285.825	-258.611	141.297
500	25.300	32.270	22.630	4.820	-285.805	-251.804	110.062
600	26.410	36.990	24.640	7.410	-285.793	-245.008	89.243
631	26.723	38.328	25.280	8.234	-285.808	-242.899	84.128
700	27.420	41.140	26.711	10.100	-285.757	-238.204	74.370
800	28.380	44.860	28.748	12.890	-285.614	-231.422	63.221
900	29.310	48.260	30.738	15.770	-285.441	-224.666	54.556
1000	30.220	51.390	32.640	18.750	-285.222	-217.917	47.625
1100	31.110	54.310	34.474	21.820	-284.971	-211.189	41.959
1156	31.608	55.872	35.482	23.571	-284.823	-207.447	39.219
1156	31.608	55.872	35.482	23.571	-285.840	-207.447	39.219
1200	32.000	57.060	36.252	24.970	-285.664	-204.466	37.238

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 21.820 + 8.600\times10^{-3}T - 2.050\times10^{5}T^{-2}$
$H°-H°_{298} = 21.820\times10^{-3}T + 4.300\times10^{-6}T^{2} + 2.050\times10^{2}T^{-1} - 7.575$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -286.989 + 2.502\times10^{-3}T - 1.858\times10^{-6}T^{2} + 181.400T^{-1}$
$\Delta Gf° = -286.989 - 2.502\times10^{-3}T\ln T + 1.858\times10^{-6}T^{2} + 90.700T^{-1} + 84.638\times10^{-3}T$
631-750 K: $\Delta Hf° = -284.440 - 5.822\times10^{-3}T + 5.167\times10^{-6}T^{2} + 122.400T^{-1}$
$\Delta Gf° = -284.440 + 5.822\times10^{-3}T\ln T - 5.167\times10^{-6}T^{2} + 61.200T^{-1} + 31.438\times10^{-3}T$
750-1156 K: $\Delta Hf° = -287.350 + 0.427\times10^{-3}T + 1.266\times10^{-6}T^{2} + 436.000T^{-1}$
$\Delta Gf° = -287.350 - 0.427\times10^{-3}T\ln T - 1.266\times10^{-6}T^{2} + 218.000T^{-1} + 73.481\times10^{-3}T$
1156-1200 K: $\Delta Hf° = -291.387 + 2.827\times10^{-3}T + 0.943\times10^{-6}T^{2} + 1218.900T^{-1}$
$\Delta Gf° = -291.387 - 2.827\times10^{-3}T\ln T - 0.943\times10^{-6}T^{2} + 609.450T^{-1} + 93.234\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Levitskii (305). Other data based on Chizhikov (91).

$Ni_4W(c)$
Tetranickel Tungsten
[Formation: $4Ni(c) + W(c) = Ni_4W(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	29.400	36.000	36.000	0	-7.500	-7.393	5.419
300	29.420	36.180	36.013	.050	-7.509	-7.395	5.387
400	30.380	44.780	37.180	3.040	-7.718	-7.334	4.007
500	31.350	51.660	39.400	6.130	-8.074	-7.199	3.147
600	32.320	57.460	41.943	9.310	-8.640	-6.990	2.546
631	32.618	59.096	42.746	10.317	-8.903	-6.891	2.387
700	33.280	62.520	44.534	12.590	-9.178	-6.644	2.074
800	34.250	67.020	47.057	15.970	-9.378	-6.274	1.714
900	35.220	71.110	49.510	19.440	-9.541	-5.878	1.427
1000	36.180	74.870	51.860	23.010	-9.664	-5.474	1.196
1100	37.150	78.370	54.115	26.680	-9.759	-5.007	.995

*Entropy at 298 K estimated.

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 26.420 + 9.778\times10^{-3}T + 0.058\times10^{5}T^{-2}$

$H°-H°_{298} = 26.420\times10^{-3}T + 4.889\times10^{-6}T^{2} - 0.058\times10^{2}T^{-1} - 8.292$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -9.652 + 8.621\times10^{-3}T - 12.602\times10^{-6}T^{2} + 209.200T^{-1}$

$\Delta Gf° = -9.652 - 8.621\times10^{-3}T\ln T + 12.602\times10^{-6}T^{2} + 104.600T^{-1} + 51.762\times10^{-3}T$

631-750 K: $\Delta Hf° = 0.544 - 24.675\times10^{-3}T + 15.498\times10^{-6}T^{2} - 26.800T^{-1}$

$\Delta Gf° = 0.544 + 24.675\times10^{-3}T\ln T - 15.498\times10^{-6}T^{2} - 13.400T^{-1} - 161.038\times10^{-3}T$

750-1100 K: $\Delta Hf° = -11.096 + 0.321\times10^{-3}T - 0.110\times10^{-6}T^{2} + 1227.600T^{-1}$

$\Delta Gf° = -11.096 - 0.321\times10^{-3}T\ln T + 0.110\times10^{-6}T^{2} + 613.800T^{-1} + 7.137\times10^{-3}T$

Source: Data from Mah (320) who estimated entropy at 298 K.

$NiWO_4(c)$
Nickel Tungstate
[Formation: $Ni(c) + W(c) + 2O_2(g) = NiWO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	27.770	28.510	28.510	0	-271.000	-245.824	180.192
300	27.860	28.680	28.513	.050	-270.999	-245.668	178.966
400	30.500	37.080	29.630	2.980	-270.732	-237.256	129.629
500	32.470	44.110	31.850	6.130	-270.360	-228.934	100.066
600	34.170	50.180	34.413	9.460	-269.940	-220.696	80.387
631	34.654	51.914	35.231	10.527	-269.813	-218.153	75.557
700	35.730	55.560	37.046	12.960	-269.420	-212.509	66.347
800	37.220	60.430	39.667	16.610	-268.735	-204.431	55.847
900	38.670	64.900	42.233	20.400	-267.962	-196.441	47.702
1000	40.090	69.050	44.710	24.340	-267.083	-188.543	41.206
1100	41.500	72.940	47.104	28.420	-266.112	-180.719	35.905
1200	42.900	76.610	49.410	32.640	-265.046	-173.011	31.509

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 26.761 + 13.606\times10^{-3}T - 2.721\times10^{5}T^{-2}$

$H°- H°_{298} = 26.761\times10^{-3}T + 6.803\times10^{-6}T^{2} + 2.721\times10^{2}T^{-1} - 9.496$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf° = -272.879 + 3.490\times10^{-3}T + 1.146\times10^{-6}T^{2} + 219.700T^{-1}$

$\Delta Gf° = -272.879 - 3.490\times10^{-3}T\ln T - 1.146\times10^{-6}T^{2} + 109.850T^{-1} + 109.734\times10^{-3}T$

631-750 K: $\Delta Hf° = -270.330 - 4.834\times10^{-3}T + 8.171\times10^{-6}T^{2} + 160.700T^{-1}$

$\Delta Gf° = -270.330 + 4.834\times10^{-3}T\ln T - 8.171\times10^{-6}T^{2} + 80.350T^{-1} + 56.534\times10^{-3}T$

750-1200 K: $\Delta Hf° = -273.240 + 1.415\times10^{-3}T + 4.269\times10^{-6}T^{2} + 474.300T^{-1}$

$\Delta Gf° = -273.240 - 1.415\times10^{-3}T\ln T - 4.269\times10^{-6}T^{2} + 237.150T^{-1} + 98.577\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Amosse (9) and Rezukhina (422). Low-temperature heat capacities and entropy at 298 K from Landee (293). High-temperature data based on Zharkova (543).

$NpBr_3$(c)
Neptunium Tribromide
[Formation: $Np(c,l) + 1.5Br_2(l,g) = NpBr_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	26.110	47.000	47.000	0	-174.600	-168.748	123.694
300	26.120	47.162	47.002	.048	-174.615	-168.711	122.904
332.6	26.361	49.869	47.153	.903	-174.878	-168.056	110.428
332.6	26.361	49.869	47.153	.903	-185.475	-168.056	110.428
400	26.860	54.777	48.035	2.697	-185.083	-164.569	89.915
500	27.600	60.850	50.010	5.420	-184.571	-159.503	69.718
553	27.992	63.650	51.185	6.893	-184.338	-156.857	61.990
553	27.992	63.650	51.185	6.893	-185.678	-156.857	61.990
600	28.340	65.948	52.253	8.217	-185.423	-154.417	56.246
700	29.080	70.372	54.532	11.088	-184.831	-149.296	46.612
800	29.820	74.303	56.762	14.033	-184.169	-144.262	39.410
849	30.183	76.087	57.826	15.503	-183.819	-141.829	36.509
849	30.183	76.087	57.826	15.503	-185.079	-141.829	36.509
900	30.560	77.861	58.911	17.055	-184.660	-139.243	33.812
912	30.613	78.266	59.163	17.422	-184.559	-138.638	33.223
912	30.613	78.266	59.163	17.422	-185.799	-138.638	33.222
1000	31.000	81.107	60.972	20.135	-185.229	-134.116	29.311

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
553 K, α - β transition point of Np; ΔH° = 1.340 kcal/mol.
849 K, β - γ transition point of Np; ΔH° = 1.260 kcal/mol.
912 K, melting point of Np; ΔH° = 1.240 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 23.900 + 7.400\times10^{-3}T$
$H°- H°_{298} = 23.900\times10^{-3}T + 3.700\times10^{-6}T^2 - 7.455$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -174.010 - 2.333\times10^{-3}T - 5.961\times10^{-6}T^2 + 189.600T^{-1}$
$\Delta Gf° = -174.010 + 2.333\times10^{-3}T\ln T + 5.961\times10^{-6}T^2 + 94.800T^{-1} + 1.512\times10^{-3}T$

332.6-553 K: $\Delta Hf° = -189.011 + 11.408\times10^{-3}T - 6.194\times10^{-6}T^2 + 142.500T^{-1}$
$\Delta Gf° = -189.011 - 11.408\times10^{-3}T\ln T + 6.194\times10^{-6}T^2 + 71.250T^{-1} + 126.544\times10^{-3}T$

553-849 K: $\Delta Hf° = -187.311 + 1.106\times10^{-3}T + 3.617\times10^{-6}T^2 - 47.100T^{-1}$
$\Delta Gf° = -187.311 - 1.106\times10^{-3}T\ln T - 3.617\times10^{-6}T^2 - 23.550T^{-1} + 64.146\times10^{-3}T$

849-912 K: $\Delta Hf° = -189.166 + 1.807\times10^{-3}T + 3.617\times10^{-6}T^2 - 47.100T^{-1}$
$\Delta Gf° = -189.166 - 1.807\times10^{-3}T\ln T - 3.617\times10^{-6}T^2 - 23.550T^{-1} + 71.058\times10^{-3}T$

912-1000 K: $\Delta Hf° = -188.444 - 0.345\times10^{-3}T + 3.617\times10^{-6}T^2 - 47.100T^{-1}$
$\Delta Gf° = -188.444 + 0.345\times10^{-3}T\ln T - 3.617\times10^{-6}T^2 - 23.550T^{-1} + 55.599\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

$NpBr_4(c)$
Neptunium Tetrabromide
[Formation: $Np(c,l) + 2Br_2(l,g) = NpBr_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	30.740	58.000	58.000	0	-184.300	-176.304	129.233
300	30.760	58.190	58.000	.057	-184.322	-176.253	128.399
332.6	31.027	61.377	58.177	1.064	-184.728	-175.356	115.224
332.6	31.027	61.377	58.177	1.064	-198.858	-175.356	115.224
400	31.580	67.152	59.217	3.174	-198.443	-170.640	93.232
500	32.400	74.287	61.541	6.373	-197.896	-163.755	71.577
553	32.835	77.572	62.921	8.102	-197.643	-160.148	63.291
553	32.835	77.572	62.921	8.102	-198.983	-160.148	63.291
600	33.220	80.266	64.176	9.654	-198.708	-156.858	57.135
700	34.040	85.449	66.853	13.017	-198.071	-149.933	46.811
800	34.860	90.048	69.470	16.462	-197.356	-143.103	39.093
849	35.262	92.132	70.719	18.180	-196.979	-139.792	35.985
849	35.262	92.132	70.719	18.180	-198.239	-139.792	35.985
900	35.680	94.201	71.991	19.989	-197.792	-136.295	33.097
912	35.778	94.674	72.286	20.418	-197.683	-135.476	32.465
912	35.778	94.674	72.286	20.418	-198.923	-135.476	32.465
1000	36.500	98.003	74.405	23.598	-198.282	-129.384	28.276

*Data except enthalpy of formation at 298 K estimated.

Phase changes:
332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
553 K, α - β transition point of Np; ΔH° = 1.340 kcal/mol.
849 K, β - γ transition point of Np; ΔH° = 1.260 kcal/mol.
912 K, melting point of Np; ΔH° = 1.240 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K:
$Cp° = 28.300 + 8.200\times10^{-3}T$
$H°-H°_{298} = 28.300\times10^{-3}T + 4.100\times10^{-6}T^2 - 8.802$

Formation equations (kcal/mol):

298.15-332.6 K:
$\Delta Hf° = -182.365 - 6.979\times10^{-3}T - 5.511\times10^{-6}T^2 + 189.600T^{-1}$
$\Delta Gf° = -182.365 + 6.979\times10^{-3}T\ln T + 5.511\times10^{-6}T^2 + 94.800T^{-1} - 22.144\times10^{-3}T$

332.6-553 K:
$\Delta Hf° = -202.366 + 11.343\times10^{-3}T - 5.821\times10^{-6}T^2 + 126.800T^{-1}$
$\Delta Gf° = -202.366 - 11.343\times10^{-3}T\ln T + 5.821\times10^{-6}T^2 + 63.400T^{-1} + 144.566\times10^{-3}T$

553-849 K:
$\Delta Hf° = -200.666 + 1.041\times10^{-3}T + 3.990\times10^{-6}T^2 - 62.800T^{-1}$
$\Delta Gf° = -200.666 - 1.041\times10^{-3}T\ln T - 3.990\times10^{-6}T^2 - 31.400T^{-1} + 82.167\times10^{-3}T$

849-912 K:
$\Delta Hf° = -202.522 + 1.742\times10^{-3}T + 3.990\times10^{-6}T^2 - 62.800T^{-1}$
$\Delta Gf° = -202.522 - 1.742\times10^{-3}T\ln T - 3.990\times10^{-6}T^2 - 31.400T^{-1} + 89.080\times10^{-3}T$

912-1000 K:
$\Delta Hf° = -201.799 - 0.410\times10^{-3}T + 3.990\times10^{-6}T^2 - 62.800T^{-1}$
$\Delta Gf° = -201.799 + 0.410\times10^{-3}T\ln T - 3.990\times10^{-6}T^2 - 31.400T^{-1} + 73.620\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

$NpCl_3$(c)
Neptunium Trichloride
[Formation: Np(c,l) + 1.5Cl_2(g) = $NpCl_3$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	24.950	38.600	38.600	0	-214.700	-198.780	145.708
300	24.970	38.754	38.601	.046	-214.689	-198.681	144.738
400	25.760	46.046	39.589	2.583	-214.152	-193.429	105.683
500	26.550	51.879	41.483	5.198	-213.704	-188.302	82.306
553	26.969	54.575	42.610	6.617	-213.510	-185.619	73.357
553	26.969	54.575	42.610	6.617	-214.850	-185.619	73.357
600	27.340	56.790	43.635	7.893	-214.629	-183.143	66.709
700	28.130	61.063	45.826	10.666	-214.113	-177.935	55.553
800	28.920	64.871	47.972	13.519	-213.529	-172.807	47.208
849	29.307	66.602	48.998	14.946	-213.217	-170.322	43.844
849	29.307	66.602	48.998	14.946	-214.477	-170.322	43.844
900	29.710	68.323	50.045	16.450	-214.098	-167.681	40.718
912	29.805	68.717	50.288	16.807	-214.006	-167.062	40.034
912	29.805	68.717	50.288	16.807	-215.246	-167.062	40.034
1000	30.500	71.494	52.033	19.461	-214.727	-162.437	35.500

*Data estimated.

Phase changes: 553 K, α - β transition point of Np; ΔH° = 1.340 kcal/mol.
849 K, β - γ transition point of Np; ΔH° = 1.260 kcal/mol.
912 K, melting point of Np; ΔH° = 1.240 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K:
$Cp^\circ = 22.600 + 7.900\times10^{-3}T$
$H^\circ - H^\circ_{298} = 22.600\times10^{-3}T + 3.950\times10^{-6}T^2 - 7.089$

Formation equations (kcal/mol):

298.15-553 K:
$\Delta Hf^\circ = -217.519 + 10.263\times10^{-3}T - 5.993\times10^{-6}T^2 + 87.150T^{-1}$
$\Delta Gf^\circ = -217.519 - 10.263\times10^{-3}T\ln T + 5.993\times10^{-6}T^2 + 43.575T^{-1} + 119.046\times10^{-3}T$

553-849 K:
$\Delta Hf^\circ = -215.820 - 0.039\times10^{-3}T + 3.818\times10^{-6}T^2 - 102.450T^{-1}$
$\Delta Gf^\circ = -215.820 + 0.039\times10^{-3}T\ln T - 3.818\times10^{-6}T^2 - 51.225T^{-1} + 56.647\times10^{-3}T$

849-912 K:
$\Delta Hf^\circ = -217.675 + 0.662\times10^{-3}T + 3.818\times10^{-6}T^2 - 102.450T^{-1}$
$\Delta Gf^\circ = -217.675 - 0.662\times10^{-3}T\ln T - 3.818\times10^{-6}T^2 - 51.225T^{-1} + 63.560\times10^{-3}T$

912-1000 K:
$\Delta Hf^\circ = -216.952 - 1.490\times10^{-3}T + 3.818\times10^{-6}T^2 - 102.450T^{-1}$
$\Delta Gf^\circ = -216.952 + 1.490\times10^{-3}T\ln T - 3.818\times10^{-6}T^2 - 51.225T^{-1} + 48.100\times10^{-3}T$

Source: Data are those estimated by Fuger (163).

$NpCl_4(c,l)$
Neptunium Tetrachloride
[Formation: $Np(c,l) + 2Cl_2(g) = NpCl_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	28.790	48.200	48.200	0	-235.200	-214.198	157.010
300	28.810	48.378	48.201	.053	-235.190	-214.068	155.947
400	29.680	56.785	49.340	2.978	-234.679	-207.107	113.156
500	30.550	63.502	51.524	5.989	-234.262	-200.264	87.534
553	31.011	66.603	52.822	7.621	-234.085	-196.669	77.724
553	31.011	66.603	52.822	7.621	-235.425	-196.669	77.724
600	31.420	69.149	54.002	9.088	-235.218	-193.383	70.439
700	32.290	74.057	56.524	12.273	-234.729	-186.449	58.211
800	33.160	78.425	58.994	15.545	-234.169	-179.591	49.061
811	33.261	78.878	59.261	15.910	-234.103	-178.840	48.194
811	42.000	98.361	59.261	31.710	-218.303	-178.840	48.194
849	42.000	100.284	61.055	33.306	-217.740	-177.005	45.564
849	42.000	100.284	61.055	33.306	-219.000	-177.005	45.564
900	42.000	102.734	63.347	35.448	-218.211	-174.504	42.375
912	42.000	103.290	63.869	35.952	-218.025	-173.923	41.678
912	42.000	103.290	63.869	35.952	-219.265	-173.923	41.678
1000	42.000	107.159	67.511	39.648	-218.098	-169.604	37.066

*Data except enthalpy of formation at 298 K and temperature of fusion estimated.

Phase changes:
553 K, α - β transition point of Np; ΔH° = 1.340 kcal/mol.
811 K, melting point of $NpCl_4$; ΔH° = 15.800 kcal/mol.
849 K, β - γ transition point of Np; ΔH° = 1.260 kcal/mol.
912 K, melting point of Np; ΔH° = 1.240 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-811 K:
$Cp° = 26.199 + 8.700\times10^{-3}T$
$H°-H°_{298} = 26.199\times10^{-3}T + 4.350\times10^{-6}T^2 - 8.198$
811-1000 K:
$Cp° = 42.000$
$H°-H°_{298} = 42.000\times10^{-3}T - 2.352$

Formation equations (kcal/mol):

298.15-553 K:
$\Delta Hf° = -237.694 + 9.448\times10^{-3}T - 5.637\times10^{-6}T^2 + 53.000T^{-1}$
$\Delta Gf° = -237.694 - 9.448\times10^{-3}T\ln T + 5.637\times10^{-6}T^2 + 26.500T^{-1} + 130.656\times10^{-3}T$
553-811 K:
$\Delta Hf° = -235.994 - 0.854\times10^{-3}T + 4.174\times10^{-6}T^2 - 136.600T^{-1}$
$\Delta Gf° = -235.994 + 0.854\times10^{-3}T\ln T - 4.174\times10^{-6}T^2 - 68.300T^{-1} + 68.257\times10^{-3}T$
811-849 K:
$\Delta Hf° = -230.148 + 14.947\times10^{-3}T - 0.176\times10^{-6}T^2 - 136.600T^{-1}$
$\Delta Gf° = -230.148 - 14.947\times10^{-3}T\ln T + 0.176\times10^{-6}T^2 - 68.300T^{-1} + 163.359\times10^{-3}T$
849-912 K:
$\Delta Hf° = -232.003 + 15.648\times10^{-3}T - 0.176\times10^{-6}T^2 - 136.600T^{-1}$
$\Delta Gf° = -232.003 - 15.648\times10^{-3}T\ln T + 0.176\times10^{-6}T^2 - 68.300T^{-1} + 170.272\times10^{-3}T$
912-1000 K:
$\Delta Hf° = -231.280 + 13.496\times10^{-3}T - 0.176\times10^{-6}T^2 - 136.600T^{-1}$
$\Delta Gf° = -231.280 - 13.496\times10^{-3}T\ln T + 0.176\times10^{-6}T^2 - 68.300T^{-1} + 154.812\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K and temperature of fusion.

$NpF_3(c)$
Neptunium Trifluoride
[Formation: $Np(c,l) + 1.5F_2(g) = NpF_3(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	23.500	29.800	29.800	0	-365.400	-349.024	255.838
300	23.520	29.945	29.802	.043	-365.391	-348.923	254.187
400	24.360	36.827	30.734	2.437	-364.904	-343.509	187.682
500	25.200	42.353	32.523	4.915	-364.520	-338.207	147.828
553	25.645	44.914	33.590	6.262	-364.366	-335.427	132.562
553	25.645	44.914	33.590	6.262	-365.706	-335.427	132.562
600	26.040	47.022	34.560	7.477	-365.521	-332.860	121.243
700	26.880	51.099	36.638	10.123	-365.087	-327.450	102.233
800	27.720	54.743	38.677	12.853	-364.590	-322.108	87.995
849	28.132	56.403	39.652	14.221	-364.321	-319.514	82.248
849	28.132	56.403	39.652	14.221	-365.581	-319.514	82.248
900	28.560	58.056	40.648	15.667	-365.247	-316.755	76.918
912	28.661	58.435	40.880	16.010	-365.165	-316.108	75.751
912	28.661	58.435	40.880	16.010	-366.405	-316.108	75.751
1000	29.400	61.109	42.544	18.565	-365.968	-311.277	68.029

*Data estimated.

Phase changes:
553 K, α - β transition point of Np; ΔH° = 1.340 kcal/mol.
849 K, β - γ transition point of Np; ΔH° = 1.260 kcal/mol.
912 K, melting point of Np; ΔH° = 1.240 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1000 K:
$Cp° = 21.000 + 8.400\times10^{-3}T$
$H°-H°_{298} = 21.000\times10^{-3}T + 4.200\times10^{-6}T^2 - 6.635$

Formation equations (kcal/mol):

298.15-553 K:
$\Delta Hf° = -367.734 + 9.141\times10^{-3}T - 5.872\times10^{-6}T^2 + 38.850T^{-1}$
$\Delta Gf° = -367.734 - 9.141\times10^{-3}T\ln T + 5.872\times10^{-6}T^2 + 19.425T^{-1} + 112.864\times10^{-3}T$

553-849 K:
$\Delta Hf° = -366.034 - 1.161\times10^{-3}T + 3.939\times10^{-6}T^2 - 150.750T^{-1}$
$\Delta Gf° = -366.034 + 1.161\times10^{-3}T\ln T - 3.939\times10^{-6}T^2 - 75.375T^{-1} + 50.466\times10^{-3}T$

849-912 K:
$\Delta Hf° = -367.889 - 0.460\times10^{-3}T + 3.939\times10^{-6}T^2 - 150.750T^{-1}$
$\Delta Gf° = -367.889 + 0.460\times10^{-3}T\ln T - 3.939\times10^{-6}T^2 - 75.375T^{-1} + 57.378\times10^{-3}T$

912-1000 K:
$\Delta Hf° = -367.167 - 2.612\times10^{-3}T + 3.939\times10^{-6}T^2 - 150.750T^{-1}$
$\Delta Gf° = -367.167 + 2.612\times10^{-3}T\ln T - 3.939\times10^{-6}T^2 - 75.375T^{-1} + 41.919\times10^{-3}T$

Source: Data are those estimated by Fuger (163).

$NpF_4(c)$
Neptunium Tetrafluoride
[Formation: $Np(c,l) + 2F_2(g) = NpF_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	27.740	36.500	36.500	0	-447.900	-426.300	312.482
300	27.760	36.672	36.502	.051	-447.890	-426.167	310.458
400	28.680	44.784	37.602	2.873	-447.360	-419.007	228.932
500	29.600	51.282	39.708	5.787	-446.942	-411.970	180.070
553	30.088	54.288	40.963	7.369	-446.772	-408.273	161.351
553	30.088	54.288	40.963	7.369	-448.112	-408.273	161.351
600	30.520	56.760	42.105	8.793	-447.913	-404.894	147.481
700	31.440	61.534	44.547	11.891	-447.451	-397.760	124.185
800	32.360	65.792	46.941	15.081	-446.925	-390.698	106.732
849	32.811	67.729	48.085	16.678	-446.641	-387.263	99.688
849	32.811	67.729	48.085	16.678	-447.901	-387.263	99.688
900	33.280	69.657	49.254	18.363	-447.550	-383.628	93.157
912	33.390	70.099	49.525	18.763	-447.464	-382.776	91.727
912	33.390	70.099	49.525	18.763	-448.704	-382.776	91.727
1000	34.200	73.211	51.474	21.737	-448.235	-376.439	82.270

*Data estimated.

Phase changes: 553 K, α - β transition point of Np; ΔH° = 1.340 kcal/mol.
849 K, β - γ transition point of Np; ΔH° = 1.260 kcal/mol.
912 K, melting point of Np; ΔH° = 1.240 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 25.000 + 9.200\times10^{-3}T$
$H^\circ - H^\circ_{298} = 25.000\times10^{-3}T + 4.600\times10^{-6}T^2 - 7.863$

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf^\circ = -450.017 + 8.887\times10^{-3}T - 5.559\times10^{-6}T^2 - 11.400T^{-1}$
$\Delta Gf^\circ = -450.017 - 8.887\times10^{-3}T\ln T + 5.559\times10^{-6}T^2 - 5.700T^{-1} + 128.588\times10^{-3}T$
553-849 K: $\Delta Hf^\circ = -448.318 - 1.415\times10^{-3}T + 4.252\times10^{-6}T^2 - 201.000T^{-1}$
$\Delta Gf^\circ = -448.318 + 1.415\times10^{-3}T\ln T - 4.252\times10^{-6}T^2 - 100.500T^{-1} + 66.190\times10^{-3}T$
849-912 K: $\Delta Hf^\circ = -450.173 - 0.714\times10^{-3}T + 4.252\times10^{-6}T^2 - 201.000T^{-1}$
$\Delta Gf^\circ = -450.173 + 0.714\times10^{-3}T\ln T - 4.252\times10^{-6}T^2 - 100.500T^{-1} + 73.102\times10^{-3}T$
912-1000 K: $\Delta Hf^\circ = -449.450 - 2.866\times10^{-3}T + 4.252\times10^{-6}T^2 - 201.000T^{-1}$
$\Delta Gf^\circ = -449.450 + 2.866\times10^{-3}T\ln T - 4.252\times10^{-6}T^2 - 100.500T^{-1} + 57.643\times10^{-3}T$

Source: Data are those estimated by Fuger (163).

NpO(g)
Neptunium Monoxide (ideal gas)
[Formation: $Np(c,l) + 0.5O_2(g) = NpO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.580	57.826	57.826	0	-1.000	-7.340	5.380
300	7.590	57.873	57.826	.014	-1.005	-7.379	5.375
400	7.960	60.109	58.129	.792	-1.337	-9.456	5.166
500	8.230	61.917	58.711	1.603	-1.779	-11.437	4.999
553	8.325	62.750	59.058	2.042	-2.075	-12.446	4.919
553	8.325	62.750	59.058	2.042	-3.415	-12.446	4.919
600	8.410	63.433	59.375	2.435	-3.641	-13.203	4.809
700	8.530	64.740	60.051	3.282	-4.124	-14.760	4.608
800	8.620	65.885	60.710	4.140	-4.605	-16.247	4.438
849	8.649	66.398	61.024	4.563	-4.841	-16.953	4.364
849	8.649	66.398	61.024	4.563	-6.101	-16.953	4.364
900	8.680	66.904	61.343	5.005	-6.312	-17.599	4.274
912	8.685	67.019	61.417	5.109	-6.361	-17.749	4.253
912	8.685	67.019	61.417	5.109	-7.601	-17.749	4.253
1000	8.720	67.820	61.945	5.875	-8.154	-18.702	4.087
1100	8.760	68.654	62.518	6.750	-8.783	-19.726	3.919
1200	8.790	69.418	63.062	7.627	-9.415	-20.694	3.769
1300	8.810	70.122	63.578	8.507	-10.049	-21.607	3.632
1400	8.830	70.775	64.069	9.389	-10.684	-22.472	3.508
1500	8.840	71.385	64.537	10.272	-11.321	-23.294	3.394
1600	8.850	71.956	64.983	11.157	-11.959	-24.070	3.288
1700	8.860	72.493	65.409	12.043	-12.599	-24.808	3.189
1800	8.870	73.000	65.817	12.930	-13.241	-25.506	3.097
1900	8.880	73.480	66.208	13.817	-13.886	-26.172	3.010
2000	8.880	73.936	66.583	14.705	-14.533	-26.802	2.929

*Data estimated.

Phase changes:
553 K, α - β transition point of Np; ΔH° = 1.340 kcal/mol.
849 K, β - γ transition point of Np; ΔH° = 1.260 kcal/mol.
912 K, melting point of Np; ΔH° = 1.240 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.459 + 0.296\times10^{-3}T - 0.860\times10^{5}T^{-2}$
$H° - H°_{298} = 8.459\times10^{-3}T + 0.148\times10^{-6}T^{2} + 0.860\times10^{2}T^{-1} - 2.824$

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf° = -2.681 + 5.747\times10^{-3}T - 9.915\times10^{-6}T^{2} + 253.000T^{-1}$
$\Delta Gf° = -2.681 - 5.747\times10^{-3}T\ln T + 9.915\times10^{-6}T^{2} + 126.500T^{-1} + 12.739\times10^{-3}T$
553-849 K: $\Delta Hf° = -0.981 - 4.555\times10^{-3}T - 0.103\times10^{-6}T^{2} + 63.400T^{-1}$
$\Delta Gf° = -0.981 + 4.555\times10^{-3}T\ln T + 0.103\times10^{-6}T^{2} + 31.700T^{-1} - 49.660\times10^{-3}T$
849-912 K: $\Delta Hf° = -2.836 - 3.854\times10^{-3}T - 0.103\times10^{-6}T^{2} + 63.400T^{-1}$
$\Delta Gf° = -2.836 + 3.854\times10^{-3}T\ln T + 0.103\times10^{-6}T^{2} + 31.700T^{-1} - 42.747\times10^{-3}T$
912-2000 K: $\Delta Hf° = -2.114 - 6.006\times10^{-3}T - 0.103\times10^{-6}T^{2} + 63.400T^{-1}$
$\Delta Gf° = -2.114 + 6.006\times10^{-3}T\ln T + 0.103\times10^{-6}T^{2} + 31.700T^{-1} - 58.207\times10^{-3}T$

Source: Data are those estimated by Pedley (396).

$Os(CO)_5(g)$
Osmium Pentacarbonyl (ideal gas)

[Formation: $Os(c) + 5C(c) + 2.5O_2(g) = Os(CO)_5(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	41.930	110.730	110.730	0	-247.000	-239.116	175.275
300	42.030	110.990	110.730	.078	-246.986	-239.067	174.158
400	46.010	123.680	112.438	4.497	-246.157	-236.553	129.245
500	48.600	134.240	115.772	9.234	-245.436	-234.239	102.385
600	50.600	143.280	119.617	14.198	-244.859	-232.050	84.523
700	52.230	151.210	123.579	19.342	-244.403	-229.957	71.795
800	53.590	158.270	127.476	24.635	-244.031	-227.917	62.263
900	54.710	164.650	131.260	30.051	-243.726	-225.928	54.862
1000	55.650	170.470	134.899	35.571	-243.458	-223.972	48.948

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 45.538 + 11.102\times10^{-3}T - 6.150\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 45.538\times10^{-3}T + 5.551\times10^{-6}T^{2} + 6.150\times10^{2}T^{-1} - 16.133$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf^\circ = -247.058 + 4.237\times10^{-3}T + 0.009\times10^{-6}T^{2} - 359.500T^{-1}$

$\Delta Gf^\circ = -247.058 - 4.237\times10^{-3}T\ln T - 0.009\times10^{-6}T^{2} - 179.750T^{-1} + 52.804\times10^{-3}T$

Source: Data from Behrens (26).

OsO(g)
Osmium Monoxide (ideal gas)
[Formation: $Os(c) + 0.5O_2(g) = OsO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.630	56.860	56.860	0	105.000	97.678	-71.599
300	7.640	56.907	56.860	.014	104.996	97.633	-71.125
400	8.020	59.160	57.165	.798	104.830	95.204	-52.016
500	8.280	60.980	57.752	1.614	104.677	92.815	-40.569
600	8.450	62.503	58.420	2.450	104.521	90.458	-32.949
700	8.560	63.815	59.099	3.301	104.361	88.128	-27.514
800	8.640	64.963	59.762	4.161	104.191	85.818	-23.444
900	8.700	65.985	60.398	5.028	104.009	83.531	-20.284
1000	8.740	66.905	61.004	5.901	103.819	81.265	-17.760
1100	8.770	67.740	61.579	6.777	103.617	79.019	-15.700
1200	8.800	68.503	62.124	7.655	103.403	76.795	-13.986
1300	8.820	69.209	62.643	8.536	103.180	74.585	-12.539
1400	8.840	69.863	63.135	9.419	102.943	72.395	-11.301
1500	8.850	70.473	63.604	10.304	102.699	70.221	-10.231
1600	8.860	71.045	64.052	11.189	102.440	68.063	-9.297
1700	8.870	71.582	64.478	12.076	102.173	65.926	-8.475
1800	8.880	72.090	64.888	12.963	101.893	63.800	-7.746
1900	8.880	72.570	65.280	13.851	101.602	61.690	-7.096
2000	8.890	73.026	65.656	14.740	101.301	59.597	-6.512

*Enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.598 + 0.188\times10^{-3}T - 0.910\times10^{5}T^{-2}$

$H° - H°_{298} = 8.598\times10^{-3}T + 0.094\times10^{-6}T^{2} + 0.910\times10^{2}T^{-1} - 2.877$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 105.020 - 0.653\times10^{-3}T - 0.612\times10^{-6}T^{2} + 68.400T^{-1}$

$\Delta Gf° = 105.020 + 0.653\times10^{-3}T\ln T + 0.612\times10^{-6}T^{2} + 34.200T^{-1} - 28.911\times10^{-3}T$

Source: Data from Pedley (396) who estimated enthalpy of formation at 298 K.

$PC(g)$
Phosphorus Monocarbide (ideal gas)
[Formation: $P(c,l,1/4P_4(g)) + C(c) = PC(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.149	51.661	51.661	0	107.500	95.434	-69.954
300	7.154	51.705	51.662	.013	107.498	95.358	-69.468
317.3	7.205	52.108	51.675	.137	107.487	94.660	-65.199
317.3	7.205	52.108	51.675	.137	107.330	94.660	-65.199
400	7.446	53.802	51.944	.743	107.208	91.373	-49.923
500	7.741	55.496	52.492	1.502	107.021	87.434	-38.217
550	7.865	56.240	52.799	1.893	106.914	85.466	-33.961
550	7.865	56.240	52.799	1.893	104.006	85.466	-33.961
600	7.989	56.930	53.115	2.289	103.975	83.783	-30.518
700	8.184	58.177	53.751	3.098	103.888	80.424	-25.109
800	8.335	59.280	54.374	3.925	103.778	77.080	-21.057
900	8.452	60.269	54.976	4.764	103.648	73.749	-17.908
1000	8.545	61.164	55.550	5.614	103.506	70.435	-15.393
1100	8.619	61.982	56.097	6.473	103.354	67.146	-13.341
1200	8.679	62.735	56.620	7.338	103.192	63.850	-11.629
1300	8.728	63.432	57.118	8.208	103.022	60.577	-10.184
1400	8.770	64.080	57.592	9.083	102.847	57.319	-8.948
1500	8.805	64.686	58.045	9.962	102.666	54.074	-7.878
1600	8.835	65.256	58.478	10.844	102.482	50.840	-6.944
1700	8.861	65.792	58.893	11.729	102.292	47.618	-6.122
1800	8.884	66.299	59.290	12.616	102.099	44.409	-5.392
1900	8.905	66.780	59.672	13.505	101.902	41.208	-4.740
2000	8.923	67.237	60.038	14.397	101.703	38.021	-4.155

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.811 + 0.688\times10^{-3}T - 0.771\times10^{5}T^{-2}$
$H°-H°_{298} = 7.811\times10^{-3}T + 0.344\times10^{-6}T^{2} + 0.771\times10^{2}T^{-1} - 2.618$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = 107.993 + 0.494\times10^{-3}T - 3.607\times10^{-6}T^{2} - 95.200T^{-1}$
$\Delta Gf° = 107.993 - 0.494\times10^{-3}T\ln T + 3.607\times10^{-6}T^{2} - 47.600T^{-1} - 39.847\times10^{-3}T$
317.3-550 K: $\Delta Hf° = 108.306 - 1.999\times10^{-3}T - 0.422\times10^{-6}T^{2} - 95.200T^{-1}$
$\Delta Gf° = 108.306 + 1.999\times10^{-3}T\ln T + 0.422\times10^{-6}T^{2} - 47.600T^{-1} - 54.183\times10^{-3}T$
550-2000 K: $\Delta Hf° = 104.846 - 0.661\times10^{-3}T - 0.426\times10^{-6}T^{2} - 195.500T^{-1}$
$\Delta Gf° = 104.846 + 0.661\times10^{-3}T\ln T + 0.426\times10^{-6}T^{2} - 97.750T^{-1} - 39.285\times10^{-3}T$

Source: Data from JANAF (127) except enthalpy of formation at 298 K converted to P(white) standard state.

PH(g)
Phosphorus Monohydride (ideal gas)
[Formation: $P(c,l,1/4P_4(g)) + 0.5H_2(g) = PH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	6.970	46.900	46.900	0	56.400	49.997	-36.648
300	6.970	46.944	46.901	.013	56.396	49.956	-36.393
317.3	6.977	47.335	46.914	.134	56.357	49.587	-34.154
317.3	6.977	47.335	46.914	.134	56.200	49.587	-34.154
400	7.008	48.953	47.175	.711	55.971	47.891	-26.166
500	7.100	50.525	47.693	1.416	55.697	45.904	-20.064
550	7.171	51.205	47.982	1.773	55.564	44.916	-17.848
550	7.171	51.205	47.982	1.773	52.656	44.916	-17.848
600	7.242	51.832	48.277	2.133	52.608	44.215	-16.105
700	7.411	52.961	48.867	2.866	52.518	42.824	-13.370
800	7.586	53.962	49.442	3.616	52.437	41.445	-11.322
900	7.756	54.865	49.995	4.383	52.367	40.076	-9.732
1000	7.914	55.691	50.525	5.166	52.306	38.713	-8.461
1100	8.057	56.452	51.029	5.965	52.255	37.356	-7.422
1200	8.188	57.159	51.512	6.777	52.210	36.003	-6.557
1300	8.308	57.819	51.971	7.602	52.171	34.654	-5.826
1400	8.417	58.439	52.411	8.439	52.140	33.308	-5.200
1500	8.519	59.023	52.833	9.285	52.110	31.963	-4.657
1600	8.615	59.576	53.237	10.142	52.087	30.621	-4.183
1700	8.706	60.101	53.626	11.008	52.066	29.281	-3.764
1800	8.792	60.601	53.999	11.883	52.050	27.941	-3.392
1900	8.874	61.078	54.359	12.767	52.036	26.604	-3.060
2000	8.954	61.536	54.707	13.658	52.027	25.264	-2.761

*Data estimated.

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 6.605 + 1.214\times10^{-3}T + 0.003\times10^{5}T^{-2}$
$H°-H°_{298} = 6.605\times10^{-3}T + 0.607\times10^{-6}T^{2} - 0.003\times10^{2}T^{-1} - 2.022$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = 56.747 - 0.422\times10^{-3}T - 2.788\times10^{-6}T^{2} + 7.950T^{-1}$
$\Delta Gf° = 56.747 + 0.422\times10^{-3}T\ln T + 2.788\times10^{-6}T^{2} + 3.975T^{-1} - 25.920\times10^{-3}T$
317.3-550 K: $\Delta Hf° = 57.060 - 2.915\times10^{-3}T + 0.398\times10^{-6}T^{2} + 7.950T^{-1}$
$\Delta Gf° = 57.060 + 2.915\times10^{-3}T\ln T - 0.398\times10^{-6}T^{2} + 3.975T^{-1} - 40.257\times10^{-3}T$
550-2000 K: $\Delta Hf° = 53.600 - 1.577\times10^{-3}T + 0.394\times10^{-6}T^{2} - 92.350T^{-1}$
$\Delta Gf° = 53.600 + 1.577\times10^{-3}T\ln T - 0.394\times10^{-6}T^{2} - 46.175T^{-1} - 25.359\times10^{-3}T$

Source: Data are those estimated by JANAF (127) except enthalpy of formation at 298 K converted to P(white) standard state.

$PH_2(g)$
Phosphorus Dihydride (ideal gas)
[Formation: $P(c,l,1/4P_4(g)) + H_2(g) = PH_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.312	50.800	50.800	0	25.900	22.986	-16.849
300	8.319	50.851	50.801	.015	25.891	22.967	-16.731
317.3	8.390	51.319	50.817	.160	25.817	22.802	-15.705
317.3	8.390	51.319	50.817	.160	25.660	22.802	-15.705
400	8.732	53.300	51.132	.867	25.273	22.104	-12.077
500	9.185	55.297	51.771	1.763	24.841	21.363	-9.338
550	9.421	56.183	52.132	2.228	24.641	21.010	-8.349
550	9.421	56.183	52.132	2.228	21.733	21.010	-8.349
600	9.656	57.013	52.505	2.705	21.627	20.950	-7.631
700	10.121	58.536	53.259	3.694	21.442	20.853	-6.511
800	10.557	59.917	54.007	4.728	21.292	20.779	-5.677
900	10.951	61.183	54.734	5.804	21.175	20.723	-5.032
1000	11.300	62.356	55.439	6.917	21.085	20.677	-4.519
1100	11.604	63.447	56.117	8.063	21.018	20.641	-4.101
1200	11.866	64.468	56.771	9.236	20.966	20.608	-3.753
1300	12.092	65.427	57.400	10.435	20.929	20.581	-3.460
1400	12.286	66.331	58.007	11.654	20.901	20.554	-3.209
1500	12.454	67.184	58.590	12.891	20.879	20.530	-2.991
1600	12.599	67.993	59.153	14.144	20.863	20.506	-2.801
1700	12.724	68.760	59.695	15.410	20.849	20.487	-2.634
1800	12.834	69.491	60.220	16.688	20.837	20.464	-2.485
1900	12.930	70.187	60.726	17.976	20.825	20.445	-2.352
2000	13.014	70.853	61.216	19.274	20.815	20.425	-2.232

*Data estimated.

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 8.687 + 2.378\times10^{-3}T - 0.963\times10^{5}T^{-2}$
$H° - H°_{298} = 8.687\times10^{-3}T + 1.189\times10^{-6}T^{2} + 0.963\times10^{2}T^{-1} - 3.019$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = 26.204 - 1.568\times10^{-3}T - 2.415\times10^{-6}T^{2} + 112.800T^{-1}$
$\Delta Gf° = 26.204 + 1.568\times10^{-3}T\ln T + 2.415\times10^{-6}T^{2} + 56.400T^{-1} - 21.080\times10^{-3}T$
317.3-550 K: $\Delta Hf° = 26.517 - 4.061\times10^{-3}T + 0.770\times10^{-6}T^{2} + 112.800T^{-1}$
$\Delta Gf° = 26.517 + 4.061\times10^{-3}T\ln T - 0.770\times10^{-6}T^{2} + 56.400T^{-1} - 35.417\times10^{-3}T$
550-2000 K: $\Delta Hf° = 23.057 - 2.723\times10^{-3}T + 0.766\times10^{-6}T^{2} + 12.500T^{-1}$
$\Delta Gf° = 23.057 + 2.723\times10^{-3}T\ln T - 0.766\times10^{-6}T^{2} + 6.250T^{-1} - 20.519\times10^{-3}T$

Source: Data are those estimated by JANAF (127) except enthalpy of formation at 298 K converted to P(white) standard state.

$PH_3(g)$
Phosphorus Trihydride (ideal gas)
[Formation: $P(c,l,1/4P_4(g)) + 1.5H_2(g) = PH_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.868	50.238	50.238	0	1.300	3.206	-2.350
300	8.887	50.293	50.240	.016	1.285	3.217	-2.343
317.3	9.077	50.797	50.256	.171	1.163	3.332	-2.295
317.3	9.077	50.797	50.256	.171	1.006	3.332	-2.295
400	9.987	52.997	50.600	.959	.411	4.013	-2.193
500	11.110	55.347	51.319	2.014	-.211	4.988	-2.180
550	11.639	56.432	51.734	2.584	-.481	5.506	-2.188
550	11.639	56.432	51.734	2.584	-3.389	5.506	-2.188
600	12.167	57.468	52.170	3.179	-3.552	6.323	-2.303
700	13.130	59.417	53.067	4.445	-3.811	7.991	-2.495
800	13.985	61.227	53.976	5.801	-3.992	9.690	-2.647
900	14.729	62.918	54.876	7.238	-4.104	11.408	-2.770
1000	15.368	64.504	55.760	8.744	-4.159	13.135	-2.871
1100	15.915	65.995	56.624	10.308	-4.172	14.864	-2.953
1200	16.380	67.401	57.464	11.924	-4.148	16.594	-3.022
1300	16.776	68.728	58.280	13.582	-4.100	18.320	-3.080
1400	17.115	69.984	59.072	15.277	-4.030	20.042	-3.129
1500	17.405	71.175	59.839	17.004	-3.945	21.758	-3.170
1600	17.655	72.306	60.583	18.757	-3.850	23.469	-3.206
1700	17.871	73.383	61.305	20.533	-3.747	25.175	-3.236
1800	18.058	74.410	62.004	22.330	-3.639	26.872	-3.263
1900	18.222	75.391	62.684	24.144	-3.528	28.564	-3.286
2000	18.365	76.329	63.342	25.974	-3.413	30.252	-3.306

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 10.761 + 4.218\times10^{-3}T - 2.801\times10^{5}T^{-2}$
$H°-H°_{298} = 10.761\times10^{-3}T + 2.109\times10^{-6}T^2 + 2.801\times10^{2}T^{-1} - 4.335$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = 1.241 - 2.722\times10^{-3}T - 1.704\times10^{-6}T^2 + 304.850T^{-1}$
$\Delta Gf° = 1.241 + 2.722\times10^{-3}T\ln T + 1.704\times10^{-6}T^2 + 152.425T^{-1} - 11.140\times10^{-3}T$
317.3-550 K: $\Delta Hf° = 1.554 - 5.215\times10^{-3}T + 1.480\times10^{-6}T^2 + 304.850T^{-1}$
$\Delta Gf° = 1.554 + 5.215\times10^{-3}T\ln T - 1.480\times10^{-6}T^2 + 152.425T^{-1} - 25.476\times10^{-3}T$
550-2000 K: $\Delta Hf° = -1.906 - 3.877\times10^{-3}T + 1.476\times10^{-6}T^2 + 204.550T^{-1}$
$\Delta Gf° = -1.906 + 3.877\times10^{-3}T\ln T - 1.476\times10^{-6}T^2 + 102.275T^{-1} - 10.579\times10^{-3}T$

Source: Data from JANAF (127) except enthalpy of formation at 298 K converted to P(white) standard state.

PN(g)
Phosphorus Mononitride (ideal gas)
[Formation: $P(c,l,1/4P_4(g)) + 0.5N_2(g) = PN(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	7.096	50.435	50.435	0	40.960	35.674	-26.149
300	7.100	50.479	50.436	.013	40.955	35.640	-25.964
317.3	7.144	50.878	50.449	.136	40.919	35.336	-24.338
317.3	7.144	50.878	50.449	.136	40.762	35.336	-24.338
400	7.355	52.555	50.717	.735	40.553	33.947	-18.548
500	7.636	54.227	51.257	1.485	40.322	32.323	-14.128
550	7.761	54.960	51.561	1.870	40.215	31.514	-12.522
550	7.761	54.960	51.561	1.870	37.307	31.514	-12.522
600	7.885	55.641	51.873	2.261	37.286	30.989	-11.287
700	8.088	56.873	52.502	3.060	37.250	29.942	-9.348
800	8.249	57.964	53.117	3.878	37.218	28.901	-7.895
900	8.376	58.943	53.711	4.709	37.188	27.863	-6.766
1000	8.478	59.831	54.279	5.552	37.158	26.829	-5.863
1100	8.559	60.643	54.821	6.404	37.129	25.797	-5.125
1200	8.625	61.391	55.339	7.263	37.099	24.767	-4.511
1300	8.680	62.083	55.830	8.129	37.069	23.743	-3.991
1400	8.726	62.728	56.300	8.999	37.038	22.718	-3.546
1500	8.765	63.332	56.749	9.874	37.007	21.695	-3.161
1600	8.799	63.898	57.178	10.752	36.974	20.677	-2.824
1700	8.828	64.433	57.590	11.633	36.941	19.658	-2.527
1800	8.853	64.938	57.984	12.517	36.908	18.643	-2.264
1900	8.876	65.417	58.362	13.404	36.875	17.630	-2.028
2000	8.897	65.873	58.727	14.292	36.840	16.618	-1.816

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.528 + 0.878\times10^{-3}T - 0.617\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 7.528\times10^{-3}T + 0.439\times10^{-6}T^{2} + 0.617\times10^{2}T^{-1} - 2.490$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf^\circ = 40.870 + 0.470\times10^{-3}T - 3.041\times10^{-6}T^{2} + 65.650T^{-1}$
$\Delta Gf^\circ = 40.870 - 0.470\times10^{-3}T\ln T + 3.041\times10^{-6}T^{2} + 32.825T^{-1} - 16.023\times10^{-3}T$
317.3-550 K: $\Delta Hf^\circ = 41.183 - 2.022\times10^{-3}T + 0.144\times10^{-6}T^{2} + 65.650T^{-1}$
$\Delta Gf^\circ = 41.183 + 2.022\times10^{-3}T\ln T - 0.144\times10^{-6}T^{2} + 32.825T^{-1} - 30.359\times10^{-3}T$
550-2000 K: $\Delta Hf^\circ = 37.723 - 0.685\times10^{-3}T + 0.140\times10^{-6}T^{2} - 34.650T^{-1}$
$\Delta Gf^\circ = 37.723 + 0.685\times10^{-3}T\ln T - 0.140\times10^{-6}T^{2} - 17.325T^{-1} - 15.461\times10^{-3}T$

Source: Data from Gurvich (194).

$P_3N_5(c)$
Triphosphorus Pentanitride
[Formation: $3P(c,l,1/4P_4(g)) + 2.5N_2(g) = P_3N_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	35.600	44.000	44.000	0	-71.400	-41.619	30.507
300	35.800	44.221	44.001	.066	-71.399	-41.437	30.186
317.3	37.565	46.278	44.070	.701	-71.363	-39.707	27.349
317.3	37.565	46.278	44.070	.701	-71.834	-39.707	27.349
400	46.000	56.017	45.539	4.191	-71.345	-31.377	17.143
500	52.000	66.963	48.747	9.108	-70.073	-21.519	9.406
550	54.000	72.027	50.635	11.766	-69.246	-16.747	6.655
550	54.000	72.027	50.635	11.766	-77.970	-16.747	6.655
600	56.000	76.813	52.620	14.516	-76.815	-11.230	4.090
700	59.000	85.684	56.721	20.274	-74.291	-.494	.154
800	61.000	93.698	60.849	26.279	-71.577	9.866	-2.695

*Entropy at 298 K estimated.

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 49.081 + 18.968x10^{-3}T - 17.011x10^{5}T^{-2}$
$H°- H°_{298} = 49.081x10^{-3}T + 9.484x10^{-6}T^{2} + 17.011x10^{2}T^{-1} - 21.182$

Formation equations (kcal/mol):

298.15-317.3 K: $ΔHf° = -83.412 + 21.392x10^{-3}T - 1.543x10^{-6}T^{2} + 1720.850T^{-1}$
$ΔGf° = -83.412 - 21.392x10^{-3}TlnT + 1.543x10^{-6}T^{2} + 860.425T^{-1} + 251.916x10^{-3}T$
317.3-550 K: $ΔHf° = -82.472 + 13.912x10^{-3}T + 8.011x10^{-6}T^{2} + 1720.850T^{-1}$
$ΔGf° = -82.472 - 13.912x10^{-3}TlnT - 8.011x10^{-6}T^{2} + 860.425T^{-1} + 208.907x10^{-3}T$
550-800 K: $ΔHf° = -92.853 + 17.926x10^{-3}T + 7.999x10^{-6}T^{2} + 1419.950T^{-1}$
$ΔGf° = -92.853 - 17.926x10^{-3}TlnT - 7.999x10^{-6}T^{2} + 709.975T^{-1} + 253.600x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data from JANAF (127) who estimated entropy at 298 K.

$POBr_3(g)$
Phosphoryl Bromide (ideal gas)

[Formation: $P(c,l,1/4P_4(g)) + 0.5O_2(g) + 1.5Br_2(l,g) = POBr_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	21.478	85.978	85.978	0	-97.000	-96.131	70.465
300	21.508	86.111	85.978	.040	-97.027	-96.125	70.026
317.3	21.726	87.323	86.018	.414	-97.281	-96.066	66.168
317.3	21.726	87.323	86.018	.414	-97.438	-96.066	66.168
332.6	21.919	88.351	86.102	.748	-97.668	-95.995	63.077
332.6	21.919	88.351	86.102	.748	-108.266	-95.995	63.077
400	22.770	92.487	86.840	2.259	-108.302	-93.508	51.090
500	23.567	97.660	88.502	4.579	-108.299	-89.809	39.255
550	23.836	99.921	89.439	5.765	-108.280	-87.974	34.957
550	23.836	99.921	89.439	5.765	-111.188	-87.974	34.957
600	24.105	102.007	90.400	6.964	-111.080	-85.868	31.277
700	24.480	105.753	92.333	9.394	-110.851	-81.684	25.503
800	24.751	109.040	94.220	11.856	-110.608	-77.534	21.181
900	24.951	111.968	96.032	14.342	-110.359	-73.415	17.827
1000	25.102	114.605	97.760	16.845	-110.105	-69.324	15.151
1100	25.218	117.003	99.402	19.361	-109.849	-65.258	12.965
1200	25.309	119.201	100.961	21.888	-109.589	-61.215	11.149
1300	25.382	121.230	102.444	24.422	-109.331	-57.196	9.615
1400	25.441	123.113	103.853	26.964	-109.071	-53.193	8.304
1500	25.489	124.870	105.197	29.510	-108.813	-49.213	7.170
1600	25.529	126.516	106.478	32.061	-108.557	-45.246	6.180
1700	25.563	128.065	107.703	34.616	-108.300	-41.298	5.309
1800	25.591	129.527	108.875	37.174	-108.046	-37.363	4.536
1900	25.615	130.911	109.998	39.734	-107.795	-33.440	3.846
2000	25.636	132.226	111.078	42.296	-107.547	-29.537	3.228

*Enthalpy of formation at 298 K estimated.

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.415 + 0.824\text{x}10^{-3}T - 2.829\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 24.415\text{x}10^{-3}T + 0.412\text{x}10^{-6}T^2 + 2.829\text{x}10^{2}T^{-1} - 8.265$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -94.596 - 10.135\text{x}10^{-3}T - 2.875\text{x}10^{-6}T^2 + 260.300T^{-1}$
$\Delta Gf° = -94.596 + 10.135\text{x}10^{-3}T\ln T + 2.875\text{x}10^{-6}T^2 + 130.150T^{-1} - 65.220\text{x}10^{-3}T$
317.3-332.6 K: $\Delta Hf° = -94.282 - 12.628\text{x}10^{-3}T + 0.311\text{x}10^{-6}T^2 + 260.300T^{-1}$
$\Delta Gf° = -94.282 + 12.628\text{x}10^{-3}T\ln T - 0.311\text{x}10^{-6}T^2 + 130.150T^{-1} - 79.557\text{x}10^{-3}T$
332.6-550 K: $\Delta Hf° = -109.283 + 1.113\text{x}10^{-3}T + 0.078\text{x}10^{-6}T^2 + 213.200T^{-1}$
$\Delta Gf° = -109.283 - 1.113\text{x}10^{-3}T\ln T - 0.078\text{x}10^{-6}T^2 + 106.600T^{-1} + 45.476\text{x}10^{-3}T$
550-2000 K: $\Delta Hf° = -112.743 + 2.451\text{x}10^{-3}T + 0.074\text{x}10^{-6}T^2 + 112.900T^{-1}$
$\Delta Gf° = -112.743 - 2.451\text{x}10^{-3}T\ln T - 0.074\text{x}10^{-6}T^2 + 56.450T^{-1} + 60.374\text{x}10^{-3}T$

Source: Enthalpy of formation at 298 K estimated. Data from JANAF (127).

$POCl_3(g)$
Phosphoryl Chloride (ideal gas)
[Formation: $P(c,l,1/4P_4(g)) + 0.5O_2(g) + 1.5Cl_2(g) = POCl_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	20.296	77.767	77.767	0	-133.480	-122.600	89.867
300	20.335	77.893	77.767	.038	-133.482	-122.533	89.264
317.3	20.619	79.041	77.805	.392	-133.499	-121.900	83.961
317.3	20.619	79.041	77.805	.392	-133.656	-121.900	83.961
400	21.979	83.988	78.588	2.160	-133.736	-118.826	64.923
500	23.007	89.011	80.185	4.413	-133.757	-115.093	50.306
550	23.349	91.224	81.089	5.574	-133.748	-113.241	44.997
550	23.349	91.224	81.089	5.574	-136.656	-113.241	44.997
600	23.690	93.270	82.020	6.750	-136.557	-111.116	40.474
700	24.163	96.960	83.897	9.144	-136.341	-106.893	33.373
800	24.500	100.209	85.737	11.578	-136.113	-102.703	28.057
900	24.748	103.110	87.509	14.041	-135.874	-98.540	23.929
1000	24.935	105.728	89.202	16.526	-135.628	-94.406	20.632
1100	25.079	108.111	90.814	19.027	-135.380	-90.295	17.940
1200	25.191	110.298	92.347	21.541	-135.128	-86.208	15.700
1300	25.280	112.318	93.807	24.064	-134.876	-82.143	13.809
1400	25.353	114.195	95.198	26.596	-134.624	-78.096	12.191
1500	25.412	115.946	96.523	29.134	-134.371	-74.068	10.792
1600	25.461	117.587	97.788	31.678	-134.120	-70.054	9.569
1700	25.502	119.132	98.999	34.226	-133.870	-66.056	8.492
1800	25.537	120.591	100.159	36.778	-133.621	-62.075	7.537
1900	25.567	121.973	101.271	39.334	-133.374	-58.105	6.684
2000	25.592	123.285	102.339	41.892	-133.131	-54.151	5.917

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.021 + 1.084\times10^{-3}T - 3.599\times10^{5}T^{-2}$
$H°-H°_{298} = 24.021\times10^{-3}T + 0.542\times10^{-6}T^{2} + 3.599\times10^{2}T^{-1} - 8.417$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -135.002 + 3.367\times10^{-3}T - 3.026\times10^{-6}T^{2} + 234.850T^{-1}$
$\Delta Gf° = -135.002 - 3.367\times10^{-3}T\ln T + 3.026\times10^{-6}T^{2} + 117.425T^{-1} + 58.554\times10^{-3}T$
317.3-550 K: $\Delta Hf° = -134.689 + 0.874\times10^{-3}T + 0.159\times10^{-6}T^{2} + 234.850T^{-1}$
$\Delta Gf° = -134.689 - 0.874\times10^{-3}T\ln T - 0.159\times10^{-6}T^{2} + 117.425T^{-1} + 44.218\times10^{-3}T$
550-2000 K: $\Delta Hf° = -138.149 + 2.211\times10^{-3}T + 0.155\times10^{-6}T^{2} + 134.550T^{-1}$
$\Delta Gf° = -138.149 - 2.211\times10^{-3}T\ln T - 0.155\times10^{-6}T^{2} + 67.275T^{-1} + 59.116\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data from JANAF (127).

$POF_3(g)$
Phosphoryl Fluoride (ideal gas)
[Formation: $P(c,l,1/4P_4(g)) + 0.5O_2(g) + 1.5F_2(g) = POF_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	16.447	68.187	68.187	0	-289.500	-277.932	203.727
300	16.499	68.289	68.189	.030	-289.509	-277.861	202.419
317.3	16.915	69.226	68.220	.319	-289.575	-277.187	190.918
317.3	16.915	69.226	68.220	.319	-289.732	-277.187	190.918
400	18.904	73.385	68.868	1.807	-290.016	-273.880	149.639
500	20.604	77.797	70.221	3.788	-290.236	-269.817	117.935
550	21.205	79.795	71.001	4.837	-290.308	-267.786	106.407
550	21.205	79.795	71.001	4.837	-293.216	-267.786	106.407
600	21.805	81.666	71.813	5.912	-293.190	-265.474	96.698
700	22.662	85.095	73.471	8.137	-293.098	-260.862	81.444
800	23.287	88.164	75.119	10.436	-292.969	-256.267	70.008
900	23.752	90.935	76.725	12.789	-292.811	-251.686	61.117
1000	24.104	93.456	78.273	15.183	-292.636	-247.126	54.009
1100	24.377	95.767	79.760	17.608	-292.447	-242.584	48.196
1200	24.591	97.898	81.185	20.056	-292.248	-238.061	43.356
1300	24.762	99.873	82.547	22.524	-292.041	-233.553	39.263
1400	24.901	101.713	83.850	25.008	-291.829	-229.063	35.758
1500	25.015	103.435	85.099	27.504	-291.615	-224.587	32.722
1600	25.110	105.053	86.297	30.010	-291.398	-220.126	30.067
1700	25.189	106.578	87.446	32.525	-291.180	-215.677	27.727
1800	25.256	108.019	88.548	35.047	-290.962	-211.240	25.648
1900	25.313	109.386	89.609	37.576	-290.744	-206.816	23.789
2000	25.362	110.686	90.631	40.110	-290.528	-202.406	22.118

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.841 + 2.388\times10^{-3}T - 5.428\times10^{5}T^{-2}$
$H°-H°_{298} = 21.841\times10^{-3}T + 1.194\times10^{-6}T^{2} + 5.428\times10^{2}T^{-1} - 8.439$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -291.013 + 1.665\times10^{-3}T - 2.504\times10^{-6}T^{2} + 369.450T^{-1}$
$\Delta Gf° = -291.013 - 1.665\times10^{-3}T\ln T + 2.504\times10^{-6}T^{2} + 184.725T^{-1} + 50.537\times10^{-3}T$
317.3-550 K: $\Delta Hf° = -290.700 - 0.828\times10^{-3}T + 0.682\times10^{-6}T^{2} + 369.450T^{-1}$
$\Delta Gf° = -290.700 + 0.828\times10^{-3}T\ln T - 0.682\times10^{-6}T^{2} + 184.725T^{-1} + 36.201\times10^{-3}T$
550-2000 K: $\Delta Hf° = -294.160 + 0.510\times10^{-3}T + 0.678\times10^{-6}T^{2} + 269.150T^{-1}$
$\Delta Gf° = -294.160 - 0.510\times10^{-3}T\ln T - 0.678\times10^{-6}T^{2} + 134.575T^{-1} + 51.098\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data from JANAF (127).

$PaBr_4(c)$
Protactinium Tetrabromide
[Formation: $Pa(c) + 2Br_2(l,g) = PaBr_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	30.400	55.800	55.800	0	-197.500	-188.747	138.353
300	30.410	55.988	55.801	.056	-197.522	-188.692	137.460
332.6	30.661	59.138	55.977	1.051	-197.919	-187.712	123.343
332.6	30.661	59.138	55.977	1.051	-212.049	-187.712	123.343
400	31.180	64.842	57.002	3.136	-211.602	-182.828	99.892
500	31.950	71.882	59.298	6.292	-210.915	-175.715	76.804
600	32.720	77.776	61.899	9.526	-210.192	-168.741	61.463
700	33.490	82.877	64.540	12.836	-209.432	-161.892	50.544
800	34.260	87.399	67.119	16.224	-208.628	-155.153	42.385
900	35.030	91.479	69.603	19.688	-207.786	-148.521	36.065
1000	35.800	95.210	71.980	23.230	-206.898	-141.983	31.030

*Data except enthalpy of formation at 298 K estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 28.100 + 7.700x10^{-3}T$
$H°- H°_{298} = 28.100x10^{-3}T + 3.850x10^{-6}T^2 - 8.720$

Formation equations (kcal/mol):

298.15-332.6 K: $ΔHf° = -193.616 - 13.793x10^{-3}T + 2.563x10^{-6}T^2 + 0.300T^{-1}$
$ΔGf° = -193.616 + 13.793x10^{-3}TlnT - 2.563x10^{-6}T^2 + 0.150T^{-1} - 61.492x10^{-3}T$
332.6-1000 K: $ΔHf° = -213.617 + 4.529x10^{-3}T + 2.253x10^{-6}T^2 - 62.500T^{-1}$
$ΔGf° = -213.617 - 4.529x10^{-3}TlnT - 2.253x10^{-6}T^2 - 31.250T^{-1} + 105.218x10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

$PaBr_5(c,l)$
Protactinium Pentabromide
[Formation: $Pa(c) + 2.5Br_2(l,g) = PaBr_5(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	38.600	69.000	69.000	0	-206.100	-195.859	143.567
300	38.630	69.239	69.002	.071	-206.124	-195.795	142.634
332.6	38.927	73.239	69.225	1.335	-206.546	-194.651	127.903
332.6	38.927	73.239	69.225	1.335	-224.209	-194.651	127.903
400	39.540	80.477	70.527	3.980	-223.496	-188.737	103.120
500	40.450	89.397	73.439	7.979	-222.407	-180.173	78.753
556	40.961	93.718	75.267	10.259	-221.776	-175.475	68.974
556	45.000	108.934	75.267	18.719	-213.316	-175.475	68.974
600	45.000	112.361	77.863	20.699	-212.642	-172.506	62.835
700	45.000	119.298	83.299	25.199	-211.138	-165.937	51.807
800	45.000	125.307	88.183	29.699	-209.670	-159.578	43.594
900	45.000	130.607	92.608	34.199	-208.241	-153.405	37.251
1000	45.000	135.349	96.650	38.699	-206.845	-147.388	32.211

*Data except enthalpy of formation at 298 K and temperature and enthalpy of fusion estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
556 K, melting point of $PaBr_5$; ΔH° = 8.460 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-556 K: $Cp° = 35.900 + 9.100\times10^{-3}T$
$H°-H°_{298} = 35.900\times10^{-3}T + 4.550\times10^{-6}T^2 - 11.108$
556-1000 K: $Cp° = 45.000$
$H°-H°_{298} = 45.000\times10^{-3}T - 6.301$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -201.912 - 15.039\times10^{-3}T + 3.313\times10^{-6}T^2 + 0.300T^{-1}$
$\Delta Gf° = -201.912 + 15.039\times10^{-3}T\ln T - 3.313\times10^{-6}T^2 + 0.150T^{-1} - 64.397\times10^{-3}T$
332.6-556 K: $\Delta Hf° = -226.913 + 7.864\times10^{-3}T + 2.925\times10^{-6}T^2 - 78.200T^{-1}$
$\Delta Gf° = -226.913 - 7.864\times10^{-3}T\ln T - 2.925\times10^{-6}T^2 - 39.100T^{-1} + 143.991\times10^{-3}T$
556-1000 K: $\Delta Hf° = -222.106 + 16.964\times10^{-3}T - 1.625\times10^{-6}T^2 - 78.200T^{-1}$
$\Delta Gf° = -222.106 - 16.964\times10^{-3}T\ln T + 1.625\times10^{-6}T^2 - 39.100T^{-1} + 190.334\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

$PaCl_4$(c)
Protactinium Tetrachloride
[Formation: Pa(c) + $2Cl_2$(g) = $PaCl_4$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	28.980	46.300	46.300	0	-249.600	-227.930	167.075
300	29.000	46.479	46.300	.054	-249.588	-227.795	165.947
400	29.900	54.945	47.447	2.999	-248.979	-220.624	120.542
500	30.800	61.714	49.646	6.034	-248.355	-213.606	93.366
600	31.700	67.409	52.144	9.159	-247.703	-206.717	75.296
700	32.600	72.363	54.686	12.374	-247.008	-199.940	62.423
800	33.500	76.775	57.176	15.679	-246.269	-193.267	52.798
900	34.400	80.773	59.580	19.074	-245.478	-186.688	45.334
1000	35.300	84.444	61.885	22.559	-244.635	-180.202	39.383

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 26.300 + 9.000\times10^{-3}T$

$H°-H°_{298} = 26.300\times10^{-3}T + 4.500\times10^{-6}T^2 - 8.241$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -250.270 + 2.935\times10^{-3}T + 2.837\times10^{-6}T^2 - 136.300T^{-1}$

$\Delta Gf° = -250.270 - 2.935\times10^{-3}T\ln T - 2.837\times10^{-6}T^2 - 68.150T^{-1} + 93.263\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

$PaCl_5(c,l)$
Protactinium Pentachloride
[Formation: $Pa(c) + 2.5Cl_2(g) = PaCl_5(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	37.200	57.000	57.000	0	-273.100	-246.676	180.816
300	37.230	57.230	57.000	.069	-273.081	-246.512	179.582
400	38.140	68.065	58.473	3.837	-272.064	-237.812	129.933
500	39.050	76.674	61.280	7.697	-271.041	-229.365	100.254
579	39.771	82.454	63.784	10.810	-270.220	-222.842	84.113
579	44.000	95.459	63.784	18.340	-262.690	-222.842	84.113
600	44.000	97.026	64.919	19.264	-262.382	-221.402	80.645
700	44.000	103.809	70.003	23.664	-260.940	-214.687	67.027
800	44.000	109.684	74.604	28.064	-259.549	-208.176	56.870
900	44.000	114.867	78.796	32.464	-258.199	-201.835	49.012
1000	44.000	119.503	82.639	36.864	-256.888	-195.645	42.758

*Data except enthalpy of formation at 298 K and temperature and enthalpy of fusion estimated.

Phase change: 579 K, melting point of $PaCl_5$; ΔH° = 7.530 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-579 K: $Cp° = 34.500 + 9.100 \times 10^{-3}T$

$H°-H°_{298} = 34.500 \times 10^{-3}T + 4.550 \times 10^{-6}T^2 - 10.691$

579-1000 K: $Cp° = 44.000$

$H°-H°_{298} = 44.000 \times 10^{-3}T - 7.136$

Formation equations (kcal/mol):

298.15-579 K: $\Delta Hf° = -274.785 + 6.722 \times 10^{-3}T + 2.843 \times 10^{-6}T^2 - 170.450T^{-1}$

$\Delta Gf° = -274.785 - 6.722 \times 10^{-3}T\ln T - 2.843 \times 10^{-6}T^2 - 85.225T^{-1} + 134.379 \times 10^{-3}T$

579-1000 K: $\Delta Hf° = -271.230 + 16.222 \times 10^{-3}T - 1.707 \times 10^{-6}T^2 - 170.450T^{-1}$

$\Delta Gf° = -271.230 - 16.222 \times 10^{-3}T\ln T + 1.707 \times 10^{-6}T^2 - 85.225T^{-1} + 186.038 \times 10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

$PaF_4(c)$
Protactinium Tetrafluoride
[Formation: $Pa(c) + 2F_2(g) = PaF_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	27.400	35.100	35.100	0	-465.000	-442.881	324.637
300	27.410	35.270	35.100	.051	-464.989	-442.744	322.535
400	28.280	43.274	36.186	2.835	-464.419	-435.416	237.897
500	29.150	49.678	38.264	5.707	-463.860	-428.229	187.176
600	30.020	55.070	40.628	8.665	-463.297	-421.157	153.404
700	30.890	59.763	43.033	11.711	-462.711	-414.179	129.311
800	31.760	63.944	45.390	14.843	-462.097	-407.288	111.265
900	32.630	67.735	47.665	18.063	-461.443	-400.473	97.247
1000	33.500	71.218	49.849	21.369	-460.751	-393.738	86.050

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 24.800 + 8.700\times10^{-3}T$

$H^\circ - H^\circ_{298} = 24.800\times10^{-3}T + 4.350\times10^{-6}T^2 - 7.781$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf^\circ = -465.168 + 2.073\times10^{-3}T + 2.515\times10^{-6}T^2 - 200.700T^{-1}$

$\Delta Gf^\circ = -465.168 - 2.073\times10^{-3}T\ln T - 2.515\times10^{-6}T^2 - 100.350T^{-1} + 88.441\times10^{-3}T$

Source: Data are those estimated by Fuger (163).

$PaI_4(c)$
Proctactinium Tetraiodide
[Formation: $Pa(c) + 2I_2(c,l,g) = PaI_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	31.920	62.000	62.000	0	-125.200	-123.436	90.480
300	31.930	62.197	62.000	.059	-125.201	-123.424	89.913
386.8	32.546	70.386	62.998	2.858	-125.403	-122.891	69.435
386.8	32.546	70.386	62.998	2.858	-132.821	-122.891	69.435
400	32.640	71.480	63.260	3.288	-132.992	-122.550	66.957
458.4	33.055	75.956	64.599	5.206	-133.732	-120.969	57.673
458.4	33.055	75.956	64.599	5.206	-153.774	-120.969	57.673
500	33.350	78.840	65.666	6.587	-153.434	-118.004	51.579
600	34.060	84.983	68.386	9.958	-152.592	-110.998	40.430
700	34.770	90.287	71.146	13.399	-151.713	-104.134	32.512
800	35.480	94.976	73.836	16.912	-150.796	-97.397	26.607
900	36.190	99.196	76.424	20.495	-149.845	-90.781	22.044
1000	36.900	103.046	78.896	24.150	-148.854	-84.269	18.417

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 29.800 + 7.100x10^{-3}T$
$H°- H°_{298} = 29.800x10^{-3}T + 3.550x10^{-6}T^2 - 9.200$

Formation equations (kcal/mol):

298.15-386.8 K: $ΔHf° = -124.623 - 1.665x10^{-3}T - 0.921x10^{-6}T^2 + 0.300T^{-1}$
$ΔGf° = -124.623 + 1.665x10^{-3}TlnT + 0.921x10^{-6}T^2 + 0.150T^{-1} - 5.783x10^{-3}T$
386.8-458.4 K: $ΔHf° = -127.533 - 14.473x10^{-3}T + 2.063x10^{-6}T^2 + 0.300T^{-1}$
$ΔGf° = -127.533 + 14.473x10^{-3}TlnT - 2.063x10^{-6}T^2 + 0.150T^{-1} - 73.414x10^{-3}T$
458.4-1000 K: $ΔHf° = -156.959 + 6.207x10^{-3}T + 1.927x10^{-6}T^2 - 30.300T^{-1}$
$ΔGf° = -156.959 - 6.207x10^{-3}TlnT - 1.927x10^{-6}T^2 - 15.150T^{-1} + 117.512x10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

$PbB_2O_4(c)$
Lead Borate
[Formation: $Pb(c,l) + 2B(\beta) + 2O_2(g) = PbB_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	25.600	31.200	31.200	0	-372.000	-346.621	254.077
300	25.700	31.359	31.202	.047	-372.001	-346.462	252.394
400	30.980	39.501	32.276	2.890	-371.855	-337.967	184.654
500	35.180	46.875	34.469	6.203	-371.483	-329.530	144.035
600	38.830	53.623	37.108	9.909	-370.930	-321.195	116.994
600.65	38.849	53.665	37.126	9.934	-370.925	-321.140	116.847
600.65	38.849	53.665	37.126	9.934	-372.072	-321.140	116.847
700	41.790	59.838	39.917	13.945	-371.359	-312.766	97.649
800	44.140	65.578	42.771	18.246	-370.470	-304.452	83.171
900	45.970	70.886	45.603	22.755	-369.439	-296.258	71.940
1000	47.420	75.807	48.380	27.427	-368.303	-288.190	62.983
1100	48.570	80.383	51.085	32.228	-367.087	-280.256	55.681
1200	49.480	84.649	53.706	37.132	-365.807	-272.403	49.611
1300	50.210	88.639	56.241	42.118	-364.488	-264.678	44.496
1400	50.830	92.383	58.690	47.170	-363.144	-257.048	40.126
1500	51.420	95.911	61.056	52.283	-361.781	-249.514	36.354
1600	51.930	99.246	63.339	57.451	-360.407	-242.116	33.071
1700	52.380	102.408	65.545	62.667	-359.023	-234.736	30.177
1800	52.800	105.414	67.677	67.926	-357.636	-227.442	27.615
1900	53.200	108.279	69.739	73.226	-356.248	-220.244	25.334
2000	53.580	111.018	71.735	78.565	-354.859	-213.151	23.292

*Data except enthalpy of formation at 298 K estimated.

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 36.182 + 10.802\times10^{-3}T - 12.269\times10^{5}T^{-2}$
$H°-H°_{298} = 36.182\times10^{-3}T + 5.401\times10^{-6}T^{2} + 12.269\times10^{2}T^{-1} - 15.383$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = -376.789 + 7.425\times10^{-3}T + 1.247\times10^{-6}T^{2} + 734.900T^{-1}$
$\Delta Gf° = -376.789 - 7.425\times10^{-3}T\ln T - 1.247\times10^{-6}T^{2} + 367.450T^{-1} + 139.727\times10^{-3}T$
600.65-2000 K: $\Delta Hf° = -377.137 + 4.861\times10^{-3}T + 3.224\times10^{-6}T^{2} + 751.500T^{-1}$
$\Delta Gf° = -377.137 - 4.861\times10^{-3}T\ln T - 3.224\times10^{-6}T^{2} + 375.750T^{-1} + 125.066\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$PbB_4O_7(c)$
Lead Diborate
[Formation: $Pb(c,l) + 4B(\beta) + 3.5O_2(g) = PbB_4O_7(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	40.200	39.900	39.900	0	-683.000	-637.458	467.264
300	40.400	40.149	39.900	.075	-683.003	-637.171	464.173
400	49.360	53.030	41.597	4.573	-682.901	-621.907	339.790
500	57.020	64.890	45.086	9.902	-682.423	-606.696	265.183
600	63.470	75.875	49.312	15.938	-681.622	-591.632	215.499
600.65	63.504	75.944	49.340	15.979	-681.616	-591.532	215.229
600.65	63.504	75.944	49.340	15.979	-682.763	-591.532	215.229
700	68.630	86.060	53.844	22.551	-681.677	-576.519	179.995
800	72.780	95.504	58.468	29.629	-680.300	-561.584	153.416
900	76.070	104.271	63.077	37.075	-678.691	-546.837	132.788
1000	78.880	112.436	67.609	44.827	-676.892	-532.283	116.329
1100	81.140	120.064	72.035	52.832	-674.939	-517.945	102.905
1200	82.940	127.205	76.338	61.040	-672.865	-503.745	91.743
1300	84.250	133.897	80.511	69.402	-670.721	-489.737	82.331
1400	85.290	140.180	84.551	77.880	-668.544	-475.896	74.290
1500	86.180	146.096	88.459	86.456	-666.349	-462.199	67.342
1600	86.860	151.680	92.237	95.109	-664.161	-448.727	61.292
1700	87.400	156.963	95.891	103.823	-661.986	-435.298	55.961
1800	87.810	161.970	99.423	112.584	-659.841	-421.976	51.234
1900	88.120	166.727	102.842	121.381	-657.737	-408.817	47.024
2000	88.370	171.253	106.150	130.206	-655.679	-395.823	43.253

*Data except enthalpy of formation at 298 K estimated.

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 56.142 + 21.468\times10^{-3}T - 19.861\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 56.142\times10^{-3}T + 10.734\times10^{-6}T^{2} + 19.861\times10^{2}T^{-1} - 24.354$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf^\circ = -688.808 + 7.094\times10^{-3}T + 4.442\times10^{-6}T^{2} + 983.300T^{-1}$

$\Delta Gf^\circ = -688.808 - 7.094\times10^{-3}T\ln T - 4.442\times10^{-6}T^{2} + 491.650T^{-1} + 208.440\times10^{-3}T$

600.65-2000 K: $\Delta Hf^\circ = -689.156 + 4.530\times10^{-3}T + 6.418\times10^{-6}T^{2} + 999.900T^{-1}$

$\Delta Gf^\circ = -689.156 - 4.530\times10^{-3}T\ln T - 6.418\times10^{-6}T^{2} + 499.950T^{-1} + 193.779\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$PbB_6O_{10}(c)$
Lead Triborate
[Formation: $Pb(c,l) + 6B(\beta) + 5O_2(g) = PbB_6O_{10}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	55.200	48.600	48.600	0	-1003.000	-937.295	687.047
300	55.400	48.942	48.602	.102	-1003.005	-936.881	682.509
400	68.400	66.696	50.933	6.305	-1002.897	-914.851	499.845
500	79.880	83.221	55.757	13.732	-1002.232	-892.890	390.277
600	89.830	98.678	61.636	22.225	-1001.057	-871.141	317.309
600.65	89.889	98.775	61.676	22.283	-1001.047	-870.998	316.913
600.65	89.889	98.775	61.676	22.283	-1002.194	-870.998	316.913
700	98.880	113.227	67.978	31.674	-1000.479	-849.417	265.197
800	106.230	126.932	74.500	41.946	-998.197	-827.983	226.191
900	111.630	139.770	81.047	52.851	-995.488	-806.861	195.930
1000	115.590	151.746	87.524	64.222	-992.486	-786.062	171.792
1100	118.420	162.904	93.876	75.931	-989.295	-765.614	152.112
1200	120.220	173.290	100.067	87.868	-986.002	-745.402	135.755
1300	121.370	182.961	106.075	99.952	-982.689	-725.479	121.962
1400	121.990	191.980	111.893	112.122	-979.411	-705.816	110.181
1500	122.320	200.409	117.516	124.339	-976.206	-686.367	100.002
1600	122.540	208.310	122.946	136.582	-973.100	-667.236	91.139
1700	122.730	215.745	128.189	148.846	-970.082	-648.178	83.328
1800	122.880	222.765	133.250	161.127	-967.161	-629.256	76.401
1900	122.990	229.411	138.137	173.420	-964.342	-610.554	70.229
2000	123.080	235.722	142.860	185.724	-961.621	-592.085	64.699

*Data except enthalpy of formation at 298 K estimated.

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 76.455 + 34.362 \times 10^{-3}T - 28.002 \times 10^{5}T^{-2}$

$H°-H°_{298} = 76.455 \times 10^{-3}T + 17.181 \times 10^{-6}T^2 + 28.002 \times 10^{2}T^{-1} - 33.714$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = -1010.215 + 7.116 \times 10^{-3}T + 8.750 \times 10^{-6}T^2 + 1286.600T^{-1}$

$\Delta Gf° = -1010.215 - 7.116 \times 10^{-3}T\ln T - 8.750 \times 10^{-6}T^2 + 643.300T^{-1} + 280.490 \times 10^{-3}T$

600.65-2000 K: $\Delta Hf° = -1010.563 + 4.552 \times 10^{-3}T + 10.727 \times 10^{-6}T^2 + 1303.200T^{-1}$

$\Delta Gf° = -1010.563 - 4.552 \times 10^{-3}T\ln T - 10.727 \times 10^{-6}T^2 + 651.600T^{-1} + 265.829 \times 10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$PbCO_3(c)$
Lead Carbonate
[Formation: $Pb(c,l) + C(c) + 1.5O_2(g) = PbCO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	20.917	31.300	31.300	0	-167.950	-150.338	110.200
300	20.970	31.430	31.300	.039	-167.947	-150.229	109.440
400	23.830	37.854	32.157	2.279	-167.658	-144.361	78.874
500	26.690	43.479	33.869	4.805	-167.211	-138.586	60.575
600	29.550	48.598	35.903	7.617	-166.601	-132.917	48.414
600.65	29.569	48.630	35.917	7.636	-166.596	-132.878	48.348
600.65	29.569	48.630	35.917	7.636	-167.743	-132.878	48.348
700	32.410	53.368	38.061	10.715	-166.967	-127.171	39.704
800	35.270	57.882	40.258	14.099	-165.964	-121.550	33.205

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp^\circ = 12.397 + 28.594\times10^{-3}T - 0.005\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.397\times10^{-3}T + 14.297\times10^{-6}T^2 + 0.005\times10^{2}T^{-1} - 4.969$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf^\circ = -166.232 - 6.817\times10^{-3}T + 11.012\times10^{-6}T^2 - 198.200T^{-1}$

$\Delta Gf^\circ = -166.232 + 6.817\times10^{-3}T\ln T - 11.012\times10^{-6}T^2 - 99.100T^{-1} + 18.864\times10^{-3}T$

600.65-800 K: $\Delta Hf^\circ = -166.580 - 9.381\times10^{-3}T + 12.990\times10^{-6}T^2 - 181.600T^{-1}$

$\Delta Gf^\circ = -166.580 + 9.381\times10^{-3}T\ln T - 12.990\times10^{-6}T^2 - 90.800T^{-1} + 4.203\times10^{-3}T$

Source: Data from Chang (74).

PbH(g)
Lead Monohydride (ideal gas)
[Formation: $Pb(c,l) + 0.5H_2(g) = PbH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.045	52.737	52.737	0	56.500	50.047	-36.685
300	7.048	52.780	52.737	.013	56.494	50.007	-36.430
400	7.244	54.833	53.015	.727	56.219	47.887	-26.164
500	7.501	56.476	53.548	1.464	55.941	45.835	-20.034
600	7.755	57.867	54.155	2.227	55.661	43.837	-15.968
600.65	7.756	57.875	54.159	2.232	55.660	43.827	-15.946
600.65	7.756	57.875	54.159	2.232	54.513	43.827	-15.946
700	7.980	59.079	54.773	3.014	54.224	42.081	-13.138
800	8.170	60.158	55.381	3.822	53.955	40.367	-11.028
900	8.328	61.129	55.966	4.647	53.712	38.685	-9.394
1000	8.461	62.014	56.527	5.487	53.487	37.024	-8.091
1100	8.574	62.826	57.064	6.338	53.277	35.380	-7.029
1200	8.672	63.576	57.575	7.201	53.082	33.774	-6.151
1300	8.761	64.274	58.065	8.072	52.892	32.159	-5.406
1400	8.843	64.926	58.531	8.953	52.712	30.576	-4.773
1500	8.921	65.539	58.978	9.841	52.532	28.998	-4.225
1600	8.997	66.117	59.406	10.737	52.355	27.416	-3.745
1700	9.072	66.665	59.818	11.640	52.181	25.889	-3.328
1800	9.146	67.185	60.212	12.551	52.010	24.346	-2.956
1900	9.220	67.682	60.593	13.470	51.842	22.814	-2.624
2000	9.294	68.157	60.959	14.395	51.675	21.288	-2.326

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.123 + 1.248\times10^{-3}T - 0.400\times10^{5}T^{-2}$
$H°-H°_{298} = 7.123\times10^{-3}T + 0.624\times10^{-6}T^{2} + 0.400\times10^{2}T^{-1} - 2.313$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = 56.604 - 0.956\times10^{-3}T - 1.350\times10^{-6}T^{2} + 89.650T^{-1}$
$\Delta Gf° = 56.604 + 0.956\times10^{-3}T\ln T + 1.350\times10^{-6}T^{2} + 44.825T^{-1} - 28.347\times10^{-3}T$
600.65-2000 K: $\Delta Hf° = 56.256 - 3.520\times10^{-3}T + 0.627\times10^{-6}T^{2} + 106.250T^{-1}$
$\Delta Gf° = 56.256 + 3.520\times10^{-3}T\ln T - 0.627\times10^{-6}T^{2} + 53.125T^{-1} - 43.008\times10^{-3}T$

Source: Data from JANAF (127).

$PbSO_4(c)$
Lead Sulfate
[Reaction: $Pb(c,l) + 0.5S_2(g) + 2O_2(g) = PbSO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	24.667	35.490	35.490	0	-235.225	-203.841	149.417
300	24.717	35.636	35.490	.044	-235.226	-203.645	148.353
400	25.867	42.733	36.443	2.516	-235.216	-193.116	105.512
500	28.388	48.772	38.318	5.227	-235.045	-182.608	79.817
600	31.033	54.180	40.518	8.197	-234.702	-172.151	62.705
600.65	31.051	54.214	40.533	8.217	-234.699	-172.082	62.612
600.65	31.051	54.214	40.533	8.217	-235.846	-172.082	62.612
700	33.735	59.167	42.831	11.435	-235.324	-161.574	50.445
800	36.469	63.849	45.168	14.945	-234.570	-151.086	41.274
900	39.220	68.304	47.493	18.730	-233.564	-140.707	34.168
1000	41.983	72.579	49.789	22.790	-232.308	-130.459	28.511
1100	44.753	76.710	52.049	27.127	-230.796	-120.350	23.911

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 11.154 + 30.862x10^{-3}T + 3.833x10^{5}T^{-2}$
$H°-H°_{298} = 11.154x10^{-3}T + 15.431x10^{-6}T^{2} - 3.833x10^{2}T^{-1} - 3.412$

Reaction equations (kcal/mol):

298.15-600.65 K: $ΔHr° = -231.096 - 12.329x10^{-3}T + 12.501x10^{-6}T^{2} - 466.450T^{-1}$
$ΔGr° = -231.096 + 12.329x10^{-3}T\ln T - 12.501x10^{-6}T^{2} - 233.225T^{-1} + 27.522x10^{-3}T$
600.65-1100 K: $ΔHr° = -231.444 - 14.893x10^{-3}T + 14.478x10^{-6}T^{2} - 449.850T^{-1}$
$ΔGr° = -231.444 + 14.893x10^{-3}T\ln T - 14.478x10^{-6}T^{2} - 224.925T^{-1} + 12.861x10^{-3}T$

Source: Data from DeKock (113).

PbSe(c,l)
Lead Selenide
[Reaction: $Pb(c,l) + 0.5Se_2(g) = PbSe(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	12.000	24.500	24.500	0	-41.250	-35.260	25.846
300	12.009	24.574	24.501	.022	-41.249	-35.223	25.660
400	12.419	28.097	24.977	1.248	-41.164	-33.226	18.154
500	12.675	30.897	25.891	2.503	-41.077	-31.253	13.661
600	12.912	33.229	26.926	3.782	-40.997	-29.299	10.672
600.65	12.914	33.243	26.932	3.790	-40.996	-29.285	10.655
600.65	12.914	33.243	26.932	3.790	-42.143	-29.285	10.655
700	13.164	35.238	27.972	5.086	-42.071	-27.163	8.481
800	13.443	37.013	28.993	6.416	-41.969	-25.035	6.839
900	13.756	38.614	29.975	7.775	-41.824	-22.928	5.568
1000	14.106	40.082	30.914	9.168	-41.637	-20.844	4.555
1100	14.495	41.444	31.809	10.598	-41.403	-18.780	3.731
1200	14.923	42.723	32.666	12.069	-41.116	-16.723	3.046
1300	15.393	43.936	33.487	13.584	-40.779	-14.715	2.474
1359	15.689	44.626	33.956	14.500	-40.555	-13.537	2.177
1359	45.494	51.050	33.956	23.230	-31.825	-13.537	2.177
1400	41.455	52.342	34.476	25.013	-30.522	-13.004	2.030
1500	31.603	54.866	35.755	28.666	-28.039	-11.848	1.726

Phase changes: 600.65 K, melting point of Pb; $\Delta H^\circ = 1.147$ kcal/mol.
1359 K, melting point of PbSe; $\Delta H^\circ = 8.730$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1359 K: $Cp^\circ = 10.884 + 3.328\times10^{-3}T + 0.110\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.884\times10^{-3}T + 1.664\times10^{-6}T^2 - 0.110\times10^{2}T^{-1} - 3.356$
1359-1500 K: $Cp^\circ = 179.379 - 98.516\times10^{-3}T$
$H^\circ - H^\circ_{298} = 179.379\times10^{-3}T - 49.258\times10^{-6}T^2 - 129.572$

Reaction equations (kcal/mol):

298.15-600.65 K: $\Delta Hr^\circ = -41.466 + 0.701\times10^{-3}T + 0.060\times10^{-6}T^2 + 0.450T^{-1}$
$\Delta Gr^\circ = -41.466 - 0.701\times10^{-3}T\ln T - 0.060\times10^{-6}T^2 + 0.225T^{-1} + 24.823\times10^{-3}T$
600.65-1359 K: $\Delta Hr^\circ = -41.814 - 1.863\times10^{-3}T + 2.036\times10^{-6}T^2 + 17.050T^{-1}$
$\Delta Gr^\circ = -41.814 + 1.863\times10^{-3}T\ln T - 2.036\times10^{-6}T^2 + 8.525T^{-1} + 10.162\times10^{-3}T$
1359-1500 K: $\Delta Hr^\circ = -168.030 + 166.632\times10^{-3}T - 48.886\times10^{-6}T^2 + 28.050T^{-1}$
$\Delta Gr^\circ = -168.030 - 166.632\times10^{-3}T\ln T + 48.886\times10^{-6}T^2 + 14.025T^{-1} + 1249.438\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Entropy and heat capacity at 298 K from Kelley (246). High-temperature data based on Rasulov (416).

PbSe(g)
Lead Selenide (ideal gas)
[Reaction: $Pb(c,l) + 0.5Se_2(g) = PbSe(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°₂₉₈)/T	H°- H°₂₉₈	ΔHr°	ΔGr°	
298.15	8.660	63.000	63.000	0	13.550	8.061	-5.909
300	8.660	63.050	63.000	.016	13.545	8.028	-5.848
400	8.780	65.570	63.345	.890	13.278	6.226	-3.402
500	8.840	67.540	63.998	1.771	12.991	4.493	-1.964
600	8.870	69.150	64.722	2.657	12.678	2.823	-1.028
600.65	8.870	69.160	64.726	2.663	12.676	2.814	-1.024
600.65	8.870	69.160	64.726	2.663	11.529	2.814	-1.024
700	8.890	70.520	65.456	3.545	11.188	1.399	-.437
800	8.900	71.710	66.166	4.435	10.850	.026	-.007
900	8.910	72.760	66.843	5.325	10.526	-1.309	.318
1000	8.920	73.700	67.484	6.216	10.212	-2.613	.571
1100	8.920	74.540	68.078	7.108	9.908	-3.875	.770
1200	8.920	75.320	68.653	8.000	9.616	-5.108	.930
1300	8.930	76.040	69.199	8.893	9.330	-6.341	1.066
1400	8.930	76.700	69.711	9.785	9.050	-7.533	1.176
1500	8.930	77.310	70.191	10.678	8.773	-8.702	1.268
1600	8.930	77.890	70.658	11.571	8.500	-9.884	1.350
1700	8.930	78.430	71.098	12.464	8.229	-10.990	1.413
1800	8.930	78.940	71.519	13.357	7.962	-12.118	1.471
1900	8.930	79.420	71.919	14.251	7.698	-13.221	1.521
2000	8.930	79.880	72.308	15.144	7.437	-14.323	1.565

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.941 - 0.250 \times 10^{5}T^{-2}$
$H° - H°_{298} = 8.941 \times 10^{-3}T + 0.250 \times 10^{2}T^{-1} - 2.750$

Reaction equations (kcal/mol):

298.15-600.65 K: $\Delta Hr° = 13.941 - 1.242 \times 10^{-3}T - 1.604 \times 10^{-6}T^{2} + 36.450T^{-1}$
$\Delta Gr° = 13.941 + 1.242 \times 10^{-3}T\ln T + 1.604 \times 10^{-6}T^{2} + 18.225T^{-1} - 27.480 \times 10^{-3}T$
600.65-2000 K: $\Delta Hr° = 13.593 - 3.806 \times 10^{-3}T + 0.373 \times 10^{-6}T^{2} + 53.050T^{-1}$
$\Delta Gr° = 13.593 + 3.806 \times 10^{-3}T\ln T - 0.373 \times 10^{-6}T^{2} + 26.525T^{-1} - 42.141 \times 10^{-3}T$

Source: Data from Mills (332).

$PbSiO_3(c)$
Lead Silicate
[Formation: $Pb(c,l) + Si(c) + 1.5O_2(g) = PbSiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	21.520	26.200	26.200	0	-273.830	-253.765	186.013
300	21.620	26.330	26.200	.040	-273.830	-253.639	184.774
400	25.080	33.090	27.090	2.400	-273.685	-246.923	134.911
500	26.860	38.890	28.890	5.000	-273.393	-240.267	105.019
600	27.980	43.900	30.983	7.750	-273.040	-233.677	85.116
600.65	27.985	43.930	30.997	7.768	-273.038	-233.632	85.007
600.65	27.985	43.930	30.997	7.768	-274.185	-233.632	85.007
700	28.790	48.280	33.151	10.590	-273.831	-226.957	70.858
800	29.440	52.160	35.285	13.500	-273.447	-220.279	60.177
900	29.990	55.660	37.360	16.470	-273.030	-213.659	51.883
1000	30.480	58.850	39.350	19.500	-272.575	-207.080	45.257

<ins>Phase change</ins>: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 27.671 + 3.476\times10^{-3}T - 6.389\times10^{5}T^{-2}$

$H°-H°_{298} = 27.671\times10^{-3}T + 1.738\times10^{-6}T^{2} + 6.389\times10^{2}T^{-1} - 10.547$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = -277.331 + 6.296\times10^{-3}T - 1.132\times10^{-6}T^{2} + 514.000T^{-1}$

$\Delta Gf° = -277.331 - 6.296\times10^{-3}T\ln T + 1.132\times10^{-6}T^{2} + 257.000T^{-1} + 111.682\times10^{-3}T$

600.65-1000 K: $\Delta Hf° = -277.678 + 3.732\times10^{-3}T + 0.845\times10^{-6}T^{2} + 530.600T^{-1}$

$\Delta Gf° = -277.678 - 3.732\times10^{-3}T\ln T - 0.845\times10^{-6}T^{2} + 265.300T^{-1} + 97.021\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from King (264). High-temperature data based on Baboian (14).

Pb_2SiO_4(c)
Dilead Silicate
[Formation: $2Pb(c,l) + Si(c) + 2O_2(g) = Pb_2SiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	32.780	44.640	44.640	0	-325.800	-299.309	219.397
300	32.890	44.840	44.640	.060	-325.799	-299.145	217.924
400	37.400	55.000	46.000	3.600	-325.472	-290.304	158.613
500	39.990	63.650	48.690	7.480	-324.930	-281.574	123.074
600	41.850	71.110	51.810	11.580	-324.298	-272.960	99.424
600.65	41.860	71.155	51.831	11.607	-324.293	-272.900	99.295
600.65	41.860	71.155	51.831	11.607	-326.587	-272.900	99.295
700	43.370	77.680	55.051	15.840	-325.931	-264.078	82.448
800	44.700	83.560	58.260	20.240	-325.180	-255.292	69.742
900	45.930	88.890	61.357	24.780	-324.312	-246.590	59.879
1000	47.090	93.790	64.360	29.430	-323.356	-238.006	52.015

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 37.851 + 9.946\times10^{-3}T - 7.089\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 37.851\times10^{-3}T + 4.973\times10^{-6}T^{2} + 7.089\times10^{2}T^{-1} - 14.105$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf^\circ = -330.218 + 8.010\times10^{-3}T + 0.088\times10^{-6}T^{2} + 602.800T^{-1}$
$\Delta Gf^\circ = -330.218 - 8.010\times10^{-3}T\ln T - 0.088\times10^{-6}T^{2} + 301.400T^{-1} + 145.941\times10^{-3}T$
600.65-1000 K: $\Delta Hf^\circ = -330.913 + 2.882\times10^{-3}T + 4.042\times10^{-6}T^{2} + 636.000T^{-1}$
$\Delta Gf^\circ = -330.913 - 2.882\times10^{-3}T\ln T - 4.042\times10^{-6}T^{2} + 318.000T^{-1} + 116.619\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from King (264). High-temperature data based on Baboian (14).

$PbTe(c)$
Lead Telluride
[Reaction: $Pb(c,l) + 0.5Te_2(g) = PbTe(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	12.200	26.300	26.300	0	-35.565	-29.565	21.671
300	12.210	26.380	26.313	.020	-35.565	-29.532	21.514
400	12.440	29.920	26.770	1.260	-35.408	-27.534	15.043
500	12.680	32.720	27.700	2.510	-35.271	-25.588	11.184
600	12.910	35.050	28.733	3.790	-35.140	-23.662	8.619
600.65	12.912	35.064	28.740	3.798	-35.139	-23.648	8.604
600.65	12.912	35.064	28.740	3.798	-36.286	-23.648	8.604
700	13.150	37.060	29.789	5.090	-36.178	-21.572	6.735
800	13.380	38.830	30.805	6.420	-36.045	-19.489	5.324
900	13.620	40.420	31.787	7.770	-35.887	-17.428	4.232
1000	13.850	41.870	32.730	9.140	-35.712	-15.397	3.365
1100	14.090	43.200	33.618	10.540	-35.508	-13.376	2.657

Phase change: 600.65 K, melting point of Pb; $\Delta H^\circ = 1.147$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp^\circ = 11.517 + 2.324\text{x}10^{-3}T - 0.009\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 11.517\text{x}10^{-3}T + 1.162\text{x}10^{-6}T^{2} + 0.009\text{x}10^{2}T^{-1} - 3.540$

Reaction equations (kcal/mol):

298.15-600.65 K: $\Delta Hr^\circ = -36.292 + 2.366\text{x}10^{-3}T - 0.899\text{x}10^{-6}T^{2} + 30.200T^{-1}$

$\Delta Gr^\circ = -36.292 - 2.366\text{x}10^{-3}T\ln T + 0.899\text{x}10^{-6}T^{2} + 15.100T^{-1} + 35.609\text{x}10^{-3}T$

600.65-1100 K: $\Delta Hr^\circ = -36.640 - 0.197\text{x}10^{-3}T + 1.078\text{x}10^{-6}T^{2} + 46.800T^{-1}$

$\Delta Gr^\circ = -36.640 + 0.197\text{x}10^{-3}T\ln T - 1.078\text{x}10^{-6}T^{2} + 23.400T^{-1} + 20.948\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (332). Entropy at 298 K from Kelley (246). Other data from Blachnik (45).

$PbTe(g)$
Lead Telluride (ideal gas)
[Reaction: $Pb(c,l) + 0.5Te_2(g) = PbTe(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	8.780	64.900	64.900	0	17.935	12.427	-9.109
300	8.780	64.950	64.900	.017	17.932	12.394	-9.029
400	8.850	67.500	65.253	.899	17.731	10.573	-5.777
500	8.880	69.480	65.908	1.786	17.505	8.808	-3.850
600	8.900	71.100	66.640	2.676	17.246	7.094	-2.584
600.65	8.900	71.110	66.645	2.682	17.245	7.085	-2.578
600.65	8.900	71.110	66.645	2.682	16.098	7.085	-2.578
700	8.910	72.470	67.376	3.566	15.799	5.617	-1.754
800	8.920	73.660	68.088	4.458	15.493	4.185	-1.143
900	8.920	74.710	68.766	5.350	15.193	2.791	-.678
1000	8.930	75.650	69.408	6.242	14.890	1.425	-.311
1100	8.930	76.500	70.014	7.135	14.587	.089	-.018
1200	8.930	77.280	70.590	8.028	14.285	-1.206	.220
1300	8.930	77.990	71.128	8.921	13.979	-2.492	.419
1400	8.930	78.660	71.650	9.814	13.667	-3.756	.586
1500	8.930	79.270	72.131	10.708	13.355	-4.983	.726
1600	8.930	79.850	72.599	11.601	13.042	-6.222	.850
1700	8.940	80.390	73.040	12.495	12.731	-7.380	.949
1800	8.940	80.900	73.462	13.388	12.420	-8.558	1.039
1900	8.940	81.380	73.863	14.282	12.113	-9.708	1.117
2000	8.940	81.840	74.252	15.175	11.807	-10.853	1.186

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.940 - 0.140\times10^{5}T^{-2}$
$H°-H°_{298} = 8.940\times10^{-3}T + 0.140\times10^{2}T^{-1} - 2.712$

Reaction equations (kcal/mol):

298.15-600.65 K: $\Delta Hr° = 18.036 - 0.211\times10^{-3}T - 2.061\times10^{-6}T^{2} + 43.300T^{-1}$
$\Delta Gr° = 18.036 + 0.211\times10^{-3}T\ln T + 2.061\times10^{-6}T^{2} + 21.650T^{-1} - 20.870\times10^{-3}T$
600.65-2000 K: $\Delta Hr° = 17.688 - 2.775\times10^{-3}T - 0.083\times10^{-6}T^{2} + 59.900T^{-1}$
$\Delta Gr° = 17.688 + 2.775\times10^{-3}T\ln T + 0.083\times10^{-6}T^{2} + 29.950T^{-1} - 35.531\times10^{-3}T$

Source: Data from Mills (332).

$PbWO_4(c)$
Lead Tungstate
[Formation: $Pb(c,l) + W(c) + 2O_2(g) = PbWO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	28.630	40.200	40.200	0	-269.400	-245.220	179.749
300	28.710	40.380	40.213	.050	-269.399	-245.073	178.533
400	31.880	49.130	41.380	3.100	-269.003	-237.015	129.497
500	33.590	56.440	43.680	6.380	-268.456	-229.080	100.130
600	34.730	62.670	46.337	9.800	-267.857	-221.265	80.595
600.65	34.736	62.708	46.354	9.823	-267.852	-221.212	80.488
600.65	34.736	62.708	46.354	9.823	-268.999	-221.212	80.488
700	35.610	68.090	49.061	13.320	-268.392	-213.350	66.610
800	36.340	72.900	51.750	16.920	-267.744	-205.536	56.149
900	36.990	77.220	54.342	20.590	-267.055	-197.793	48.030
1000	37.580	81.140	56.830	24.310	-266.340	-190.140	41.555
1100	38.140	84.750	59.205	28.100	-265.580	-182.552	36.269

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 33.481 + 4.656\times10^{-3}T - 5.547\times10^{5}T^{-2}$
$H°-H°_{298} = 33.481\times10^{-3}T + 2.328\times10^{-6}T^{2} + 5.547\times10^{2}T^{-1} - 12.050$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = -273.444 + 8.355\times10^{-3}T - 0.813\times10^{-6}T^{2} + 484.700T^{-1}$
$\Delta Gf° = -273.444 - 8.355\times10^{-3}T\ln T + 0.813\times10^{-6}T^{2} + 242.350T^{-1} + 139.300\times10^{-3}T$
600.65-1100 K: $\Delta Hf° = -273.792 + 5.791\times10^{-3}T + 1.164\times10^{-6}T^{2} + 501.300T^{-1}$
$\Delta Gf° = -273.792 - 5.791\times10^{-3}T\ln T - 1.164\times10^{-6}T^{2} + 250.650T^{-1} + 124.639\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Dellien (114). Low-temperature heat capacities and entropy at 298 K from Weller (520). High-temperature data based on Zharkova (542).

$PdO(g)$
Palladium Monoxide (ideal gas)
[Formation: $Pd(c,l) + 0.5O_2(g) = PdO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.570	57.196	57.196	0	58.500	51.440	-37.706
300	7.580	57.243	57.196	.014	58.496	51.396	-37.442
400	8.000	59.484	57.499	.794	58.293	49.060	-26.805
500	8.240	61.295	58.083	1.606	58.097	46.775	-20.445
600	8.400	62.813	58.748	2.439	57.895	44.529	-16.219
700	8.520	64.121	59.424	3.288	57.684	42.318	-13.212
800	8.610	65.268	60.085	4.146	57.458	40.136	-10.965
900	8.680	66.287	60.718	5.012	57.222	37.987	-9.224
1000	8.730	67.205	61.322	5.883	56.969	35.862	-7.838
1100	8.770	68.038	61.895	6.757	56.702	33.765	-6.708
1200	8.800	68.802	62.440	7.635	56.420	31.692	-5.772
1300	8.820	69.507	62.956	8.516	56.124	29.643	-4.983
1400	8.840	70.161	63.448	9.398	55.812	27.618	-4.311
1500	8.850	70.770	63.916	10.281	55.484	25.614	-3.732
1600	8.860	71.341	64.362	11.166	55.142	23.634	-3.228
1700	8.860	71.878	64.789	12.052	54.785	21.678	-2.787
1800	8.870	72.385	65.197	12.939	54.412	19.740	-2.397
1827	8.870	72.517	65.304	13.178	54.308	19.221	-2.299
1827	8.870	72.517	65.304	13.178	50.338	19.221	-2.299
1900	8.870	72.865	65.588	13.827	49.999	17.985	-2.069
2000	8.870	73.322	65.965	14.715	49.532	16.310	-1.782
2100	8.880	73.754	66.324	15.604	49.062	14.664	-1.526
2200	8.890	74.169	66.672	16.493	48.590	13.033	-1.295
2300	8.900	74.564	67.006	17.383	48.116	11.429	-1.086
2400	8.920	74.943	67.329	18.273	47.640	9.844	-.896
2500	8.950	75.306	67.641	19.163	47.161	8.278	-.724

*Enthalpy of formation at 298 K estimated.

Phase change: 1827 K, melting point Pd; ΔH° = 3.970 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 8.571 + 0.196\times10^{-3}T - 0.941\times10^{5}T^{-2}$
$H°- H°_{298} = 8.571\times10^{-3}T + 0.098\times10^{-6}T^{2} + 0.941\times10^{2}T^{-1} - 2.880$

Formation equations (kcal/mol):

298.15-1827 K: $\Delta Hf° = 58.627 - 0.916\times10^{-3}T - 0.805\times10^{-6}T^{2} + 65.000T^{-1}$
$\Delta Gf° = 58.627 + 0.916\times10^{-3}T\ln T + 0.805\times10^{-6}T^{2} + 32.500T^{-1} - 29.930\times10^{-3}T$
1827-2000 K: $\Delta Hf° = 58.305 - 4.104\times10^{-3}T - 0.153\times10^{-6}T^{2} + 71.500T^{-1}$
$\Delta Gf° = 58.305 + 4.104\times10^{-3}T\ln T + 0.153\times10^{-6}T^{2} + 35.750T^{-1} - 52.508\times10^{-3}T$
2000-2500 K: $\Delta Hf° = 58.973 - 4.659\times10^{-3}T - 0.007\times10^{-6}T^{2} - 220.900T^{-1}$
$\Delta Gf° = 58.973 + 4.659\times10^{-3}T\ln T + 0.007\times10^{-6}T^{2} - 110.450T^{-1} - 56.730\times10^{-3}T$

Source: Data from Pedley (396) who estimated enthalpy of formation at 298 K.

$PdTe_2(c)$
Palladium Ditelluride
[Reaction: $Pd(c) + Te_2(g) = PdTe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	18.310	30.250	30.250	0	-51.330	-39.215	28.745
300	18.320	30.360	30.260	.030	-51.327	-39.144	28.516
400	18.800	35.700	30.975	1.890	-50.974	-35.132	19.195
500	19.280	39.950	32.370	3.790	-50.613	-31.218	13.645
600	19.760	43.500	33.917	5.750	-50.224	-27.359	9.965
700	20.240	46.590	35.519	7.750	-49.824	-23.587	7.364
800	20.720	49.320	37.083	9.790	-49.414	-19.874	5.429
900	21.200	51.790	38.579	11.890	-48.971	-16.206	3.935
1000	21.680	54.050	40.020	14.030	-48.519	-12.596	2.753

*Data except heat capacity and entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 16.880 + 4.800 \times 10^{-3}T$

$H° - H°_{298} = 16.880 \times 10^{-3}T + 2.400 \times 10^{-6}T^2 - 5.246$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta Hr° = -52.048 + 2.409 \times 10^{-3}T + 1.156 \times 10^{-6}T^2 - 30.700T^{-1}$

$\Delta Gr° = -52.048 - 2.409 \times 10^{-3}T\ln T - 1.156 \times 10^{-6}T^2 - 15.350T^{-1} + 57.284 \times 10^{-3}T$

Source: Data from Mills (332) who estimated all except heat capacity and entropy at 298 K.

$PrFeO_3(c)$
Praseodymium Ferrite
[Formation: $Pr(c) + Fe(c) + 1.5O_2(g) = PrFeO_3(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	24.820	22.400	22.400	0	-329.000	-306.550	224.704
300	24.870	22.550	22.400	.050	-328.993	-306.405	223.213
400	27.140	30.020	23.395	2.650	-328.751	-298.911	163.315
500	29.310	36.310	25.350	5.480	-328.393	-291.481	127.404
600	31.450	41.850	27.667	8.510	-327.962	-284.156	103.502
700	33.560	46.850	30.050	11.760	-327.452	-276.888	86.447
800	35.660	51.470	32.445	15.220	-326.879	-269.707	73.680
900	37.760	55.790	34.790	18.900	-326.259	-262.579	63.762
1000	39.850	59.880	37.100	22.780	-325.687	-255.542	55.848

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 19.050 + 20.840\times10^{-3}T - 0.390\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.050\times10^{-3}T + 10.420\times10^{-6}T^{2} + 0.390\times10^{2}T^{-1} - 6.737$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf^\circ = -331.261 + 4.256\times10^{-3}T + 0.931\times10^{-6}T^{2} + 271.000T^{-1}$

$\Delta Gf^\circ = -331.261 - 4.256\times10^{-3}T\ln T - 0.931\times10^{-6}T^{2} + 135.500T^{-1} + 105.882\times10^{-3}T$

Source: Data based on Kaul (237).

PrO(g)
Praseodymium Monoxide (ideal gas)
[Formation: Pr(c,l) + $0.5O_2$(g) = PrO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.560	59.988	59.988	0	-34.000	-39.312	28.816
300	7.570	60.035	59.988	.014	-34.005	-39.345	28.662
400	7.950	62.268	60.291	.791	-34.250	-41.087	22.448
500	8.220	64.072	60.872	1.600	-34.500	-42.766	18.693
600	8.400	65.588	61.535	2.432	-34.776	-44.399	16.172
700	8.530	66.894	62.210	3.279	-35.096	-45.978	14.355
800	8.610	68.038	62.868	4.136	-35.462	-47.508	12.978
900	8.670	69.056	63.500	5.000	-35.882	-48.982	11.894
1000	8.720	69.972	64.102	5.870	-36.357	-50.414	11.018
1068	8.747	70.548	64.495	6.464	-36.717	-51.366	10.511
1068	8.747	70.548	64.495	6.464	-37.474	-51.366	10.511
1100	8.760	70.806	64.675	6.744	-37.623	-51.781	10.288
1200	8.780	71.570	65.218	7.622	-38.088	-53.047	9.661
1204	8.781	71.599	65.239	7.657	-38.106	-53.090	9.637
1204	8.781	71.599	65.239	7.657	-39.752	-53.090	9.637
1300	8.810	72.273	65.734	8.501	-40.306	-54.133	9.100
1400	8.820	72.927	66.225	9.383	-40.883	-55.177	8.613
1500	8.840	73.536	66.692	10.266	-41.462	-56.176	8.185
1600	8.850	74.107	67.138	11.151	-42.043	-57.143	7.805
1700	8.860	74.645	67.564	12.037	-42.625	-58.058	7.464
1800	8.870	75.150	67.971	12.923	-43.210	-58.958	7.158
1900	8.880	75.630	68.362	13.810	-43.797	-59.809	6.880
2000	8.880	76.086	68.737	14.698	-44.386	-60.631	6.625

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1068 K, α - β transition point of Pr; ΔH° = 0.757 kcal/mol.
1204 K, melting point of Pr; ΔH° = 1.646 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.491 + 0.268\times10^{-3}T - 0.899\times10^{5}T^{-2}$
$H°- H°_{298} = 8.491\times10^{-3}T + 0.134\times10^{-6}T^{2} + 0.899\times10^{2}T^{-1} - 2.845$

Formation equations (kcal/mol):

298.15-1068 K: $\Delta Hf° = -34.428 + 0.706\times10^{-3}T - 2.781\times10^{-6}T^{2} + 138.600T^{-1}$
$\Delta Gf° = -34.428 - 0.706\times10^{-3}T\ln T + 2.781\times10^{-6}T^{2} + 69.300T^{-1} - 13.965\times10^{-3}T$
1068-1204 K: $\Delta Hf° = -32.795 - 4.314\times10^{-3}T - 0.117\times10^{-6}T^{2} + 67.300T^{-1}$
$\Delta Gf° = -32.795 + 4.314\times10^{-3}T\ln T + 0.117\times10^{-6}T^{2} + 33.650T^{-1} - 47.627\times10^{-3}T$
1204-2000 K: $\Delta Hf° = -33.140 - 5.394\times10^{-3}T - 0.117\times10^{-6}T^{2} + 67.300T^{-1}$
$\Delta Gf° = -33.140 + 5.394\times10^{-3}T\ln T + 0.117\times10^{-6}T^{2} + 33.650T^{-1} - 55.001\times10^{-3}T$

Source: Data from Pedley (396) who estimated all except enthalpy of formation at 298 K.

PtO(g)
Platinum Monoxide (ideal gas)
[Formation: Pt(c,l) + $0.5O_2$(g) = PtO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.540	56.625	56.625	0	101.000	94.389	-69.188
300	7.540	56.672	56.625	.014	100.996	94.349	-68.732
400	7.940	58.902	56.927	.790	100.791	92.163	-50.355
500	8.230	60.706	57.508	1.599	100.596	90.030	-39.352
600	8.420	62.221	58.169	2.431	100.398	87.936	-32.030
700	8.550	63.531	58.845	3.280	100.194	85.874	-26.811
800	8.650	64.679	59.504	4.140	99.979	83.842	-22.904
900	8.720	65.703	60.137	5.009	99.752	81.838	-19.873
1000	8.780	66.624	60.740	5.884	99.512	79.862	-17.454
1100	8.820	67.463	61.314	6.764	99.258	77.909	-15.479
1200	8.860	68.232	61.859	7.648	98.992	75.980	-13.838
1300	8.890	68.943	62.377	8.536	98.711	74.072	-12.453
1400	8.920	69.603	62.870	9.426	98.417	72.188	-11.269
1500	8.940	70.219	63.340	10.319	98.109	70.326	-10.246
1600	8.960	70.797	63.788	11.214	97.789	68.483	-9.354
1700	8.980	71.340	64.216	12.111	97.454	66.664	-8.570
1800	9.000	71.855	64.627	13.010	97.106	64.859	-7.875
1900	9.010	72.341	65.020	13.910	96.743	63.078	-7.256
2000	9.030	72.804	65.398	14.812	96.369	61.317	-6.700
2042	9.034	72.992	65.552	15.191	96.205	60.581	-6.484
2042	9.034	72.992	65.552	15.191	91.509	60.581	-6.484
2100	9.040	73.245	65.761	15.716	91.290	59.706	-6.214
2200	9.050	73.666	66.111	16.620	90.908	58.211	-5.783

Phase change: 2042 K, melting point of Pt; ΔH° = 4.696 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 8.452 + 0.346\text{x}10^{-3}T - 0.902\text{x}10^{5}T^{-2}$

$H° - H°_{298} = 8.452\text{x}10^{-3}T + 0.173\text{x}10^{-6}T^{2} + 0.902\text{x}10^{2}T^{-1} - 2.838$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 101.138 - 0.989\text{x}10^{-3}T - 0.709\text{x}10^{-6}T^{2} + 65.600T^{-1}$

$\Delta Gf° = 101.138 + 0.989\text{x}10^{-3}T\ln T + 0.709\text{x}10^{-6}T^{2} + 32.800T^{-1} - 28.850\text{x}10^{-3}T$

2000-2042 K: $\Delta Hf° = 101.806 - 1.544\text{x}10^{-3}T - 0.562\text{x}10^{-6}T^{2} - 226.800T^{-1}$

$\Delta Gf° = 101.806 + 1.544\text{x}10^{-3}T\ln T + 0.562\text{x}10^{-6}T^{2} - 113.400T^{-1} - 33.072\text{x}10^{-3}T$

2042-2200 K: $\Delta Hf° = 99.534 - 4.018\text{x}10^{-3}T + 0.068\text{x}10^{-6}T^{2} - 224.800T^{-1}$

$\Delta Gf° = 99.534 + 4.018\text{x}10^{-3}T\ln T - 0.068\text{x}10^{-6}T^{2} - 112.400T^{-1} - 49.529\text{x}10^{-3}T$

Source: Data from Pedley (396).

$PuC_{0.82}$(c)
Plutonium Carbide
[Formation: Pu(c,l) + 0.82C(c) = $PuC_{0.82}$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.009	16.632	16.632	0	-11.000	-11.622	8.519
300	11.027	16.701	16.634	.020	-10.998	-11.627	8.470
395	11.584	19.822	17.037	1.100	-10.913	-11.840	6.551
395	11.584	19.822	17.037	1.100	-11.733	-11.840	6.551
400	11.613	19.968	17.073	1.158	-11.727	-11.842	6.470
480	11.835	22.107	17.741	2.096	-11.659	-11.873	5.406
480	11.835	22.107	17.741	2.096	-11.794	-11.873	5.406
500	11.890	22.591	17.925	2.333	-11.783	-11.877	5.191
588	12.143	24.537	18.772	3.390	-11.774	-11.894	4.421
588	12.143	24.537	18.772	3.390	-11.914	-11.894	4.421
600	12.178	24.783	18.890	3.536	-11.913	-11.893	4.332
700	12.587	26.689	19.870	4.773	-11.912	-11.890	3.712
730	12.759	27.221	20.162	5.153	-11.908	-11.889	3.559
730	12.759	27.221	20.162	5.153	-11.928	-11.889	3.559
752	12.886	27.599	20.373	5.434	-11.917	-11.888	3.455
752	12.886	27.599	20.373	5.434	-12.357	-11.888	3.455
800	13.162	28.405	20.831	6.059	-12.312	-11.860	3.240
900	13.925	29.997	21.761	7.412	-12.181	-11.811	2.868
913	14.050	30.198	21.880	7.594	-12.159	-11.806	2.826
913	14.050	30.198	21.880	7.594	-12.834	-11.806	2.826
1000	14.887	31.513	22.662	8.851	-12.818	-11.708	2.559
1100	16.056	32.985	23.534	10.396	-12.712	-11.593	2.303
1200	17.434	34.439	24.382	12.069	-12.490	-11.508	2.096
1300	19.025	35.896	25.211	13.890	-12.130	-11.441	1.923
1400	20.829	37.371	26.027	15.881	-11.608	-11.406	1.781
1500	22.849	38.876	26.834	18.063	-10.902	-11.415	1.663

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 6.589 + 8.762\times10^{-3}T + 1.607\times10^{5}T^{-2}$
$H°-H°_{298} = 6.589\times10^{-3}T + 4.381\times10^{-6}T^{2} - 1.607\times10^{2}T^{-1} - 1.815$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf° = -9.660 - 0.286\times10^{-3}T - 2.721\times10^{-6}T^{2} - 301.986T^{-1}$
$\Delta Gf° = -9.660 + 0.286\times10^{-3}T\ln T + 2.721\times10^{-6}T^{2} - 150.993T^{-1} - 7.322\times10^{-3}T$
395-480 K: $\Delta Hf° = -10.271 - 2.353\times10^{-3}T + 1.169\times10^{-6}T^{2} - 301.986T^{-1}$
$\Delta Gf° = -10.271 + 2.353\times10^{-3}T\ln T - 1.169\times10^{-6}T^{2} - 150.993T^{-1} - 16.598\times10^{-3}T$
480-588 K: $\Delta Hf° = -10.666 - 1.398\times10^{-3}T + 0.311\times10^{-6}T^{2} - 301.986T^{-1}$
$\Delta Gf° = -10.666 + 1.398\times10^{-3}T\ln T - 0.311\times10^{-6}T^{2} - 150.993T^{-1} - 10.290\times10^{-3}T$
588-730 K: $\Delta Hf° = -9.777 - 5.173\times10^{-3}T + 3.753\times10^{-6}T^{2} - 301.986T^{-1}$
$\Delta Gf° = -9.777 + 5.173\times10^{-3}T\ln T - 3.753\times10^{-6}T^{2} - 150.993T^{-1} - 33.851\times10^{-3}T$
730-752 K: $\Delta Hf° = -10.072 - 4.796\times10^{-3}T + 3.753\times10^{-6}T^{2} - 301.986T^{-1}$
$\Delta Gf° = -10.072 + 4.796\times10^{-3}T\ln T - 3.753\times10^{-6}T^{2} - 150.993T^{-1} - 30.961\times10^{-3}T$
752-913 K: $\Delta Hf° = -10.713 - 4.528\times10^{-3}T + 3.753\times10^{-6}T^{2} - 301.986T^{-1}$
$\Delta Gf° = -10.713 + 4.528\times10^{-3}T\ln T - 3.753\times10^{-6}T^{2} - 150.993T^{-1} - 28.333\times10^{-3}T$
913-1500 K: $\Delta Hf° = -9.683 - 6.396\times10^{-3}T + 3.753\times10^{-6}T^{2} - 301.986T^{-1}$
$\Delta Gf° = -9.683 + 6.396\times10^{-3}T\ln T - 3.753\times10^{-6}T^{2} - 150.993T^{-1} - 42.195\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Johnson (224). Other data from Oetting (358).

$PuC_{0.88}(c)$
Plutonium Carbide
[Formation: $Pu(c,l) + 0.88C(c) = PuC_{0.88}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.400	17.380	17.380	0	-11.400	-12.221	8.958
300	11.420	17.450	17.380	.021	-11.398	-12.226	8.907
395	11.838	20.671	17.803	1.133	-11.294	-12.508	6.920
395	11.838	20.671	17.803	1.133	-12.114	-12.508	6.920
400	11.860	20.820	17.840	1.192	-12.108	-12.513	6.837
480	11.916	22.983	18.518	2.144	-12.041	-12.599	5.736
480	11.916	22.983	18.518	2.144	-12.176	-12.599	5.736
500	11.930	23.470	18.706	2.382	-12.168	-12.617	5.515
588	12.009	25.407	19.567	3.434	-12.184	-12.696	4.719
588	12.009	25.407	19.567	3.434	-12.324	-12.696	4.719
600	12.020	25.650	19.687	3.578	-12.328	-12.703	4.627
700	12.260	27.510	20.667	4.790	-12.377	-12.757	3.983
730	12.404	28.028	20.959	5.160	-12.391	-12.773	3.824
730	12.404	28.028	20.959	5.160	-12.411	-12.773	3.824
752	12.510	28.399	21.174	5.433	-12.414	-12.785	3.716
752	12.510	28.399	21.174	5.433	-12.854	-12.785	3.716
800	12.740	29.180	21.631	6.039	-12.841	-12.782	3.492
900	13.480	30.740	22.574	7.349	-12.783	-12.795	3.107
913	13.614	30.934	22.692	7.525	-12.771	-12.795	3.063
913	13.614	30.934	22.692	7.525	-13.446	-12.795	3.063
1000	14.510	32.190	23.444	8.746	-13.492	-12.708	2.777
1100	15.800	33.630	24.304	10.259	-13.450	-12.621	2.508
1200	17.380	35.090	25.161	11.915	-13.277	-12.586	2.292
1300	19.240	36.540	25.968	13.744	-12.942	-12.524	2.105
1400	21.420	38.050	26.782	15.775	-12.413	-12.518	1.954
1500	23.850	39.600	27.576	18.036	-11.662	-12.537	1.827
1600	26.600	41.230	28.382	20.557	-10.656	-12.632	1.725
1700	29.660	42.930	29.185	23.367	-9.368	-12.790	1.644
1800	32.980	44.720	30.000	26.496	-7.766	-13.040	1.583

Phase changes:
395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 1.790 + 13.934\times10^{-3}T + 4.849\times10^{5}T^{-2}$
$H°- H°_{298} = 1.790\times10^{-3}T + 6.967\times10^{-6}T^{2} - 4.849\times10^{2}T^{-1} + 0.473$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf° = -7.670 - 5.296\times10^{-3}T - 0.181\times10^{-6}T^{2} - 636.524T^{-1}$
$\Delta Gf° = -7.670 + 5.296\times10^{-3}T\ln T + 0.181\times10^{-6}T^{2} - 318.262T^{-1} - 41.910\times10^{-3}T$
395-480 K: $\Delta Hf° = -8.281 - 7.363\times10^{-3}T + 3.709\times10^{-6}T^{2} - 636.524T^{-1}$
$\Delta Gf° = -8.281 + 7.363\times10^{-3}T\ln T - 3.709\times10^{-6}T^{2} - 318.262T^{-1} - 51.187\times10^{-3}T$
480-588 K: $\Delta Hf° = -8.676 - 6.408\times10^{-3}T + 2.851\times10^{-6}T^{2} - 636.524T^{-1}$
$\Delta Gf° = -8.676 + 6.408\times10^{-3}T\ln T - 2.851\times10^{-6}T^{2} - 318.262T^{-1} - 44.878\times10^{-3}T$
588-730 K: $\Delta Hf° = -7.787 - 10.183\times10^{-3}T + 6.293\times10^{-6}T^{2} - 636.524T^{-1}$
$\Delta Gf° = -7.787 + 10.183\times10^{-3}T\ln T - 6.293\times10^{-6}T^{2} - 318.262T^{-1} - 68.439\times10^{-3}T$
730-752 K: $\Delta Hf° = -8.082 - 9.806\times10^{-3}T + 6.293\times10^{-6}T^{2} - 636.524T^{-1}$
$\Delta Gf° = -8.082 + 9.806\times10^{-3}T\ln T - 6.293\times10^{-6}T^{2} - 318.262T^{-1} - 65.549\times10^{-3}T$
752-913 K: $\Delta Hf° = -8.723 - 9.538\times10^{-3}T + 6.293\times10^{-6}T^{2} - 636.524T^{-1}$
$\Delta Gf° = -8.723 + 9.538\times10^{-3}T\ln T - 6.293\times10^{-6}T^{2} - 318.262T^{-1} - 62.921\times10^{-3}T$
913-1800 K: $\Delta Hf° = -7.693 - 11.406\times10^{-3}T + 6.293\times10^{-6}T^{2} - 636.524T^{-1}$
$\Delta Gf° = -7.693 + 11.406\times10^{-3}T\ln T - 6.293\times10^{-6}T^{2} - 318.262T^{-1} - 76.784\times10^{-3}T$

Source: Data from Tetenbaum (491).

$PuC_2(c)$
Plutonium Dicarbide
[Formation: $Pu(c,l) + 2C(c) = PuC_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.150	24.100	24.100	0	-6.800	-9.166	6.719
300	13.170	24.181	24.101	.024	-6.799	-9.182	6.689
395	14.795	28.029	24.594	1.357	-6.732	-9.947	5.503
395	14.795	28.029	24.594	1.357	-7.552	-9.947	5.503
400	14.880	28.216	24.639	1.431	-7.547	-9.977	5.451
480	15.856	31.023	25.474	2.663	-7.477	-10.471	4.768
480	15.856	31.023	25.474	2.663	-7.612	-10.471	4.768
500	16.100	31.675	25.709	2.983	-7.600	-10.591	4.629
588	16.822	34.343	26.805	4.433	-7.587	-11.118	4.132
588	16.822	34.343	26.805	4.433	-7.727	-11.118	4.132
600	16.920	34.684	26.959	4.635	-7.726	-11.187	4.075
700	17.680	37.351	28.257	6.366	-7.731	-11.764	3.673
730	17.860	38.097	28.646	6.899	-7.732	-11.937	3.574
730	17.860	38.097	28.646	6.899	-7.752	-11.937	3.574
752	17.992	38.629	28.930	7.293	-7.747	-12.063	3.506
752	17.992	38.629	28.930	7.293	-8.187	-12.063	3.506
800	18.280	39.751	29.546	8.164	-8.160	-12.311	3.363
900	18.850	41.938	30.802	10.022	-8.099	-12.836	3.117
913	18.911	42.209	30.963	10.267	-8.090	-12.904	3.089
913	18.911	42.209	30.963	10.267	-8.765	-12.904	3.089
1000	19.320	43.949	32.018	11.931	-8.864	-13.293	2.905
1100	19.720	45.810	33.189	13.883	-8.970	-13.711	2.724
1200	20.080	47.541	34.313	15.873	-9.066	-14.159	2.579
1300	20.400	49.161	35.393	17.898	-9.151	-14.580	2.451
1400	20.700	50.684	36.432	19.953	-9.224	-14.995	2.341
1500	20.960	52.122	37.431	22.036	-9.287	-15.406	2.245
1600	21.180	53.482	38.392	24.144	-9.337	-15.809	2.159
1700	21.350	54.771	39.318	26.270	-9.385	-16.216	2.085
1800	21.520	55.996	40.210	28.414	-9.425	-16.614	2.017
1900	21.670	57.164	41.072	30.574	-9.459	-17.013	1.957
2000	21.780	58.278	41.905	32.746	-9.493	-17.409	1.902
2100	21.880	59.343	42.710	34.929	-9.524	-17.806	1.853
2200	21.980	60.363	43.489	37.122	-9.553	-18.199	1.808
2300	22.080	61.343	44.245	39.325	-9.580	-18.589	1.766
2400	22.160	62.284	44.977	41.537	-9.608	-18.982	1.729
2500	22.240	63.190	45.687	43.758	-9.631	-19.371	1.693

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 17.031 + 2.424\times10^{-3}T - 4.092\times10^{5}T^{-2}$
$H°-H°_{298} = 17.031\times10^{-3}T + 1.212\times10^{-6}T^{2} + 4.092\times10^{2}T^{-1} - 6.558$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf° = -8.203 + 6.005\times10^{-3}T - 6.794\times10^{-6}T^{2} + 64.600T^{-1}$
$\Delta Gf° = -8.203 - 6.005\times10^{-3}T\ln T + 6.794\times10^{-6}T^{2} + 32.300T^{-1} + 28.595\times10^{-3}T$
395-480 K: $\Delta Hf° = -8.814 + 3.938\times10^{-3}T - 2.904\times10^{-6}T^{2} + 64.600T^{-1}$
$\Delta Gf° = -8.814 - 3.938\times10^{-3}T\ln T + 2.904\times10^{-6}T^{2} + 32.300T^{-1} + 19.319\times10^{-3}T$
480-588 K: $\Delta Hf° = -9.209 + 4.893\times10^{-3}T - 3.762\times10^{-6}T^{2} + 64.600T^{-1}$
$\Delta Gf° = -9.209 - 4.893\times10^{-3}T\ln T + 3.762\times10^{-6}T^{2} + 32.300T^{-1} + 25.627\times10^{-3}T$
588-730 K: $\Delta Hf° = -8.320 + 1.118\times10^{-3}T - 0.320\times10^{-6}T^{2} + 64.600T^{-1}$
$\Delta Gf° = -8.320 - 1.118\times10^{-3}T\ln T + 0.320\times10^{-6}T^{2} + 32.300T^{-1} + 2.066\times10^{-3}T$
730-752 K: $\Delta Hf° = -8.615 + 1.495\times10^{-3}T - 0.320\times10^{-6}T^{2} + 64.600T^{-1}$
$\Delta Gf° = -8.615 - 1.495\times10^{-3}T\ln T + 0.320\times10^{-6}T^{2} + 32.300T^{-1} + 4.956\times10^{-3}T$
752-913 K: $\Delta Hf° = -9.256 + 1.763\times10^{-3}T - 0.320\times10^{-6}T^{2} + 64.600T^{-1}$
$\Delta Gf° = -9.256 - 1.763\times10^{-3}T\ln T + 0.320\times10^{-6}T^{2} + 32.300T^{-1} + 7.584\times10^{-3}T$
913-2000 K: $\Delta Hf° = -8.226 - 0.105\times10^{-3}T - 0.320\times10^{-6}T^{2} + 64.600T^{-1}$
$\Delta Gf° = -8.226 + 0.105\times10^{-3}T\ln T + 0.320\times10^{-6}T^{2} + 32.300T^{-1} - 6.278\times10^{-3}T$
2000-2500 K: $\Delta Hf° = -4.242 - 4.351\times10^{-3}T + 0.944\times10^{-6}T^{2} - 1030.800T^{-1}$
$\Delta Gf° = -4.242 + 4.351\times10^{-3}T\ln T - 0.944\times10^{-6}T^{2} - 515.400T^{-1} - 37.879\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Campbell (67). Other data are those estimated by Oetting (356).

Pu_2C_3(c)
Diplutonium Tricarbide
[Formation: $2Pu(c,l) + 3C(c) = Pu_2C_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	27.247	35.851	35.851	0	-40.500	-41.959	30.757
300	27.302	36.020	35.853	.050	-40.492	-41.970	30.575
395	29.011	43.799	36.860	2.741	-40.103	-42.498	23.514
395	29.011	43.799	36.860	2.741	-41.743	-42.498	23.514
400	29.101	44.164	36.949	2.886	-41.722	-42.509	23.225
480	29.724	49.533	38.611	5.243	-41.442	-42.694	19.439
480	29.724	49.533	38.611	5.243	-41.712	-42.694	19.439
500	29.880	50.750	39.072	5.839	-41.662	-42.737	18.680
588	30.390	55.634	41.194	8.491	-41.553	-42.938	15.959
588	30.390	55.634	41.194	8.491	-41.833	-42.938	15.959
600	30.460	56.249	41.489	8.856	-41.824	-42.959	15.647
700	31.125	60.993	43.944	11.934	-41.794	-43.153	13.473
730	31.385	62.305	44.672	12.872	-41.791	-43.210	12.936
730	31.385	62.305	44.672	12.872	-41.831	-43.210	12.936
752	31.576	63.235	45.200	13.562	-41.817	-43.250	12.569
752	31.576	63.235	45.200	13.562	-42.697	-43.250	12.569
800	31.992	65.202	46.342	15.088	-42.635	-43.289	11.826
900	33.117	69.033	48.654	18.341	-42.489	-43.384	10.535
913	33.301	69.509	48.948	18.773	-42.466	-43.397	10.388
913	33.301	69.509	48.948	18.773	-43.816	-43.397	10.388
1000	34.530	72.593	50.873	21.720	-43.951	-43.349	9.474
1100	36.249	75.962	53.001	25.257	-44.006	-43.254	8.594
1200	38.282	79.201	55.050	28.981	-43.916	-43.220	7.871
1300	40.637	82.356	57.030	32.924	-43.643	-43.174	7.258
1400	43.318	85.463	58.949	37.119	-43.145	-43.153	6.736
1500	46.326	88.553	60.820	41.599	-42.389	-43.178	6.291

Phase changes:
395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $C_p^\circ = 23.147 + 12.306\times10^{-3}T + 0.383\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 23.147\times10^{-3}T + 6.153\times10^{-6}T^2 - 0.383\times10^{2}T^{-1} - 7.320$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = -39.205 + 4.613\times10^{-3}T - 9.093\times10^{-6}T^2 - 555.200T^{-1}$
$\Delta Gf^\circ = -39.205 - 4.613\times10^{-3}T\ln T + 9.093\times10^{-6}T^2 - 277.600T^{-1} + 17.456\times10^{-3}T$
395-480 K: $\Delta Hf^\circ = -40.426 + 0.479\times10^{-3}T - 1.313\times10^{-6}T^2 - 555.200T^{-1}$
$\Delta Gf^\circ = -40.426 - 0.479\times10^{-3}T\ln T + 1.313\times10^{-6}T^2 - 277.600T^{-1} - 1.097\times10^{-3}T$
480-588 K: $\Delta Hf^\circ = -41.217 + 2.389\times10^{-3}T - 3.029\times10^{-6}T^2 - 555.200T^{-1}$
$\Delta Gf^\circ = -41.217 - 2.389\times10^{-3}T\ln T + 3.029\times10^{-6}T^2 - 277.600T^{-1} + 11.520\times10^{-3}T$
588-730 K: $\Delta Hf^\circ = -39.438 - 5.161\times10^{-3}T + 3.855\times10^{-6}T^2 - 555.200T^{-1}$
$\Delta Gf^\circ = -39.438 + 5.161\times10^{-3}T\ln T - 3.855\times10^{-6}T^2 - 277.600T^{-1} - 35.602\times10^{-3}T$
730-752 K: $\Delta Hf^\circ = -40.028 - 4.407\times10^{-3}T + 3.855\times10^{-6}T^2 - 555.200T^{-1}$
$\Delta Gf^\circ = -40.028 + 4.407\times10^{-3}T\ln T - 3.855\times10^{-6}T^2 - 277.600T^{-1} - 29.822\times10^{-3}T$
752-913 K: $\Delta Hf^\circ = -41.311 - 3.871\times10^{-3}T + 3.855\times10^{-6}T^2 - 555.200T^{-1}$
$\Delta Gf^\circ = -41.311 + 3.871\times10^{-3}T\ln T - 3.855\times10^{-6}T^2 - 277.600T^{-1} - 24.566\times10^{-3}T$
913-1500 K: $\Delta Hf^\circ = -39.251 - 7.607\times10^{-3}T + 3.855\times10^{-6}T^2 - 555.200T^{-1}$
$\Delta Gf^\circ = -39.251 + 7.607\times10^{-3}T\ln T - 3.855\times10^{-6}T^2 - 277.600T^{-1} - 52.291\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (222). Other data from Oetting (358).

PuN(c)
Plutonium Nitride
[Formation: $Pu(c,l) + 0.5N_2(g) = PuN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.855	15.490	15.490	0	-71.510	-65.304	47.869
300	11.862	15.563	15.490	.022	-71.509	-65.266	47.545
395	12.212	18.872	15.921	1.166	-71.503	-63.291	35.018
395	12.212	18.872	15.921	1.166	-72.323	-63.291	35.018
400	12.230	19.026	15.958	1.227	-72.320	-63.177	34.518
480	12.525	21.282	16.664	2.217	-72.277	-61.353	27.934
480	12.525	21.282	16.664	2.217	-72.412	-61.353	27.934
500	12.599	21.795	16.859	2.468	-72.401	-60.893	26.616
588	12.923	23.862	17.756	3.591	-72.370	-58.871	21.881
588	12.923	23.862	17.756	3.591	-72.510	-58.871	21.881
600	12.967	24.124	17.881	3.746	-72.504	-58.592	21.342
700	13.336	26.151	18.921	5.061	-72.441	-56.278	17.571
730	13.446	26.713	19.230	5.463	-72.415	-55.586	16.641
730	13.446	26.713	19.230	5.463	-72.435	-55.586	16.641
752	13.527	27.114	19.455	5.759	-72.407	-55.079	16.007
752	13.527	27.114	19.455	5.759	-72.847	-55.079	16.007
800	13.704	27.956	19.940	6.413	-72.769	-53.947	14.738
900	14.073	29.591	20.922	7.802	-72.583	-51.605	12.531
913	14.121	29.793	21.047	7.985	-72.556	-51.303	12.280
913	14.121	29.793	21.047	7.985	-73.231	-51.303	12.280
1000	14.441	31.093	21.865	9.226	-73.204	-49.213	10.755
1100	14.810	32.487	22.768	10.691	-73.145	-46.817	9.302
1200	15.179	33.791	23.633	12.190	-73.056	-44.427	8.091
1300	15.547	35.021	24.463	13.726	-72.936	-42.047	7.069
1400	15.916	36.186	25.258	15.299	-72.783	-39.675	6.193
1500	16.284	37.297	26.024	16.909	-72.598	-37.317	5.437
1600	16.653	38.360	26.763	18.556	-72.379	-34.972	4.777

Phase changes:
395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp^\circ = 10.756 + 3.686\text{x}10^{-3}T$
$H^\circ - H^\circ_{298} = 10.756\text{x}10^{-3}T + 1.843\text{x}10^{-6}T^2 - 3.371$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = -72.131 + 3.507\text{x}10^{-3}T - 4.925\text{x}10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf^\circ = -72.131 - 3.507\text{x}10^{-3}T\ln T + 4.925\text{x}10^{-6}T^2 + 1.975T^{-1} + 41.392\text{x}10^{-3}T$
395-480 K: $\Delta Hf^\circ = -72.742 + 1.440\text{x}10^{-3}T - 1.036\text{x}10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf^\circ = -72.742 - 1.440\text{x}10^{-3}T\ln T + 1.036\text{x}10^{-6}T^2 + 1.975T^{-1} + 32.116\text{x}10^{-3}T$
480-588 K: $\Delta Hf^\circ = -73.137 + 2.395\text{x}10^{-3}T - 1.894\text{x}10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf^\circ = -73.137 - 2.395\text{x}10^{-3}T\ln T + 1.894\text{x}10^{-6}T^2 + 1.975T^{-1} + 38.424\text{x}10^{-3}T$
588-730 K: $\Delta Hf^\circ = -72.248 - 1.380\text{x}10^{-3}T + 1.548\text{x}10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf^\circ = -72.248 + 1.380\text{x}10^{-3}T\ln T - 1.548\text{x}10^{-6}T^2 + 1.975T^{-1} + 14.863\text{x}10^{-3}T$
730-752 K: $\Delta Hf^\circ = -72.543 - 1.003\text{x}10^{-3}T + 1.548\text{x}10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf^\circ = -72.543 + 1.003\text{x}10^{-3}T\ln T - 1.548\text{x}10^{-6}T^2 + 1.975T^{-1} + 17.753\text{x}10^{-3}T$
752-913 K: $\Delta Hf^\circ = -73.184 - 0.735\text{x}10^{-3}T + 1.548\text{x}10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf^\circ = -73.184 + 0.735\text{x}10^{-3}T\ln T - 1.548\text{x}10^{-6}T^2 + 1.975T^{-1} + 20.381\text{x}10^{-3}T$
913-1600 K: $\Delta Hf^\circ = -72.154 - 2.603\text{x}10^{-3}T + 1.548\text{x}10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf^\circ = -72.154 + 2.603\text{x}10^{-3}T\ln T - 1.548\text{x}10^{-6}T^2 + 1.975T^{-1} + 6.519\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (223). Other data from Oetting (357).

$PuO(g)$
Plutonium Monoxide (ideal gas)
[Formation: $Pu(c,l) + 0.5O_2(g) = PuO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.580	58.096	58.096	0	-29.000	-35.015	25.666
300	7.590	58.143	58.096	.014	-29.007	-35.052	25.535
395	7.942	60.279	58.375	.752	-29.412	-36.911	20.422
395	7.942	60.279	58.375	.752	-30.232	-36.911	20.422
400	7.960	60.379	58.399	.792	-30.252	-36.996	20.213
480	8.176	61.852	58.854	1.439	-30.562	-38.314	17.445
480	8.176	61.852	58.854	1.439	-30.697	-38.314	17.445
500	8.230	62.187	58.981	1.603	-30.777	-38.631	16.885
588	8.388	63.533	59.564	2.334	-31.155	-39.982	14.860
588	8.388	63.533	59.564	2.334	-31.295	-39.982	14.860
600	8.410	63.703	59.645	2.435	-31.347	-40.158	14.627
700	8.530	65.010	60.321	3.282	-31.777	-41.594	12.986
730	8.557	65.369	60.522	3.538	-31.905	-42.012	12.578
730	8.557	65.369	60.522	3.538	-31.925	-42.012	12.578
752	8.577	65.623	60.666	3.727	-32.011	-42.315	12.298
752	8.577	65.623	60.666	3.727	-32.451	-42.315	12.298
800	8.620	66.155	60.980	4.140	-32.626	-42.939	11.730
900	8.680	67.174	61.613	5.005	-32.992	-44.207	10.735
913	8.685	67.299	61.693	5.118	-33.039	-44.369	10.621
913	8.685	67.299	61.693	5.118	-33.714	-44.369	10.621
1000	8.720	68.090	62.215	5.875	-34.195	-45.360	9.913
1100	8.760	68.924	62.788	6.750	-34.750	-46.450	9.229
1200	8.790	69.688	63.332	7.627	-35.307	-47.490	8.649
1300	8.810	70.392	63.848	8.507	-35.865	-48.483	8.151
1400	8.830	71.045	64.339	9.389	-36.425	-49.431	7.716
1500	8.840	71.655	64.807	10.272	-36.986	-50.342	7.335
1600	8.850	72.226	65.253	11.157	-37.550	-51.213	6.995
1700	8.860	72.763	65.679	12.043	-38.115	-52.050	6.691
1800	8.870	73.270	66.087	12.930	-38.682	-52.853	6.417
1900	8.880	73.750	66.478	13.817	-39.252	-53.626	6.168
2000	8.880	74.206	66.854	14.705	-39.824	-54.369	5.941

Phase changes:
395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.459 + 0.296\times10^{-3}T - 0.860\times10^{5}T^{-2}$
$H°-H°_{298} = 8.459\times10^{-3}T + 0.148\times10^{-6}T^{2} + 0.860\times10^{2}T^{-1} - 2.824$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf° = -28.883 + 0.854\times10^{-3}T - 6.577\times10^{-6}T^{2} + 63.400T^{-1}$
$\Delta Gf° = -28.883 - 0.854\times10^{-3}T\ln T + 6.577\times10^{-6}T^{2} + 31.700T^{-1} - 18.019\times10^{-3}T$
395-480 K: $\Delta Hf° = -29.493 - 1.213\times10^{-3}T - 2.688\times10^{-6}T^{2} + 63.400T^{-1}$
$\Delta Gf° = -29.493 + 1.213\times10^{-3}T\ln T + 2.688\times10^{-6}T^{2} + 31.700T^{-1} - 27.296\times10^{-3}T$
480-588 K: $\Delta Hf° = -29.889 - 0.258\times10^{-3}T - 3.546\times10^{-6}T^{2} + 63.400T^{-1}$
$\Delta Gf° = -29.889 + 0.258\times10^{-3}T\ln T + 3.546\times10^{-6}T^{2} + 31.700T^{-1} - 20.987\times10^{-3}T$
588-730 K: $\Delta Hf° = -28.999 - 4.033\times10^{-3}T - 0.103\times10^{-6}T^{2} + 63.400T^{-1}$
$\Delta Gf° = -28.999 + 4.033\times10^{-3}T\ln T + 0.103\times10^{-6}T^{2} + 31.700T^{-1} - 44.548\times10^{-3}T$
730-752 K: $\Delta Hf° = -29.294 - 3.656\times10^{-3}T - 0.103\times10^{-6}T^{2} + 63.400T^{-1}$
$\Delta Gf° = -29.294 + 3.656\times10^{-3}T\ln T + 0.103\times10^{-6}T^{2} + 31.700T^{-1} - 41.658\times10^{-3}T$
752-913 K: $\Delta Hf° = -29.936 - 3.388\times10^{-3}T - 0.103\times10^{-6}T^{2} + 63.400T^{-1}$
$\Delta Gf° = -29.936 + 3.388\times10^{-3}T\ln T + 0.103\times10^{-6}T^{2} + 31.700T^{-1} - 39.030\times10^{-3}T$
913-2000 K: $\Delta Hf° = -28.905 - 5.256\times10^{-3}T - 0.103\times10^{-6}T^{2} + 63.400T^{-1}$
$\Delta Gf° = -28.905 + 5.256\times10^{-3}T\ln T + 0.103\times10^{-6}T^{2} + 31.700T^{-1} - 52.893\times10^{-3}T$

Source: Data from Pedley (396) who estimated some molecular constants.

PuOBr(c)
Plutonium Oxybromide
[Formation: $Pu(c,l) + 0.5O_2(g) + 0.5Br_2(l,g) = PuOBr(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	20.990	28.500	28.500	0	-207.200	-198.967	145.845
300	21.000	28.630	28.500	.039	-207.199	-198.916	144.909
332.6	21.186	30.806	28.621	.727	-207.185	-198.017	130.114
332.6	21.186	30.806	28.621	.727	-210.717	-198.017	130.114
395	21.542	34.478	29.265	2.059	-210.421	-195.663	108.257
395	21.542	34.478	29.265	2.059	-211.241	-195.663	108.257
400	21.570	34.749	29.332	2.167	-211.214	-195.467	106.797
480	22.026	38.723	30.574	3.911	-210.780	-192.357	87.581
480	22.026	38.723	30.574	3.911	-210.915	-192.357	87.581
500	22.140	39.624	30.918	4.353	-210.805	-191.587	83.741
588	22.650	43.254	32.499	6.324	-210.335	-188.244	69.966
588	22.650	43.254	32.499	6.324	-210.475	-188.244	69.966
600	22.720	43.712	32.719	6.596	-210.408	-187.790	68.402
700	23.290	47.257	34.548	8.896	-209.831	-184.066	57.467
730	23.461	48.238	35.091	9.597	-209.649	-182.966	54.776
730	23.461	48.238	35.091	9.597	-209.669	-182.966	54.776
752	23.586	48.936	35.485	10.115	-209.524	-182.162	52.940
752	23.586	48.936	35.485	10.115	-209.964	-182.162	52.940
800	23.860	50.404	36.336	11.254	-209.629	-180.399	49.282
900	24.430	53.247	38.060	13.668	-208.895	-176.789	42.930
913	24.504	53.598	38.279	13.986	-208.795	-176.326	42.208
913	24.504	53.598	38.279	13.986	-209.470	-176.326	42.208
1000	25.000	55.850	39.710	16.140	-208.946	-173.190	37.850
1100	25.570	58.260	41.289	18.668	-208.298	-169.647	33.705
1200	26.140	60.509	42.797	21.254	-207.598	-166.162	30.262
1300	26.710	62.624	44.242	23.896	-206.846	-162.741	27.359
1400	27.280	64.624	45.627	26.596	-206.042	-159.376	24.879
1500	27.850	66.526	46.958	29.352	-205.184	-156.074	22.740

*Data except enthalpy of formation at 298 K estimated.

Phase changes:
332.6 K, boiling point of Br_2 ΔH° = 7.065 kcal/mol.
395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 19.293 + 5.706\text{x}10^{-3}T - 0.004\text{x}10^{5}T^{-2}$
$H°- H°_{298} = 19.293\text{x}10^{-3}T + 2.853\text{x}10^{-6}T^{2} + 0.004\text{x}10^{2}T^{-1} - 6.007$

Formation equations (kcal/mol):

298.15-332.6 K: $ΔHf° = -207.574 + 2.642\text{x}10^{-3}T - 3.822\text{x}10^{-6}T^{2} - 22.200T^{-1}$
$ΔGf° = -207.574 - 2.642\text{x}10^{-3}T\ln T + 3.822\text{x}10^{-6}T^{2} - 11.100T^{-1} + 42.906\text{x}10^{-3}T$
332.6-395 K: $ΔHf° = -212.574 + 7.223\text{x}10^{-3}T - 3.900\text{x}10^{-6}T^{2} - 37.900T^{-1}$
$ΔGf° = -212.574 - 7.223\text{x}10^{-3}T\ln T + 3.900\text{x}10^{-6}T^{2} - 18.950T^{-1} + 84.584\text{x}10^{-3}T$
395-480 K: $ΔHf° = -213.184 + 5.156\text{x}10^{-3}T - 0.010\text{x}10^{-6}T^{2} - 37.900T^{-1}$
$ΔGf° = -213.184 - 5.156\text{x}10^{-3}T\ln T + 0.010\text{x}10^{-6}T^{2} - 18.950T^{-1} + 75.307\text{x}10^{-3}T$
480-588 K: $ΔHf° = -213.580 + 6.111\text{x}10^{-3}T - 0.868\text{x}10^{-6}T^{2} - 37.900T^{-1}$
$ΔGf° = -213.580 - 6.111\text{x}10^{-3}T\ln T + 0.868\text{x}10^{-6}T^{2} - 18.950T^{-1} + 81.616\text{x}10^{-3}T$
588-730 K: $ΔHf° = -212.690 + 2.336\text{x}10^{-3}T + 2.574\text{x}10^{-6}T^{2} - 37.900T^{-1}$
$ΔGf° = -212.690 - 2.336\text{x}10^{-3}T\ln T - 2.574\text{x}10^{-6}T^{2} - 18.950T^{-1} + 58.055\text{x}10^{-3}T$
730-752 K: $ΔHf° = -212.986 + 2.713\text{x}10^{-3}T + 2.574\text{x}10^{-6}T^{2} - 37.900T^{-1}$
$ΔGf° = -212.986 - 2.713\text{x}10^{-3}T\ln T - 2.574\text{x}10^{-6}T^{2} - 18.950T^{-1} + 60.945\text{x}10^{-3}T$
752-913 K: $ΔHf° = -213.627 + 2.981\text{x}10^{-3}T + 2.574\text{x}10^{-6}T^{2} - 37.900T^{-1}$
$ΔGf° = -213.627 - 2.981\text{x}10^{-3}T\ln T - 2.574\text{x}10^{-6}T^{2} - 18.950T^{-1} + 63.573\text{x}10^{-3}T$
913-1500 K: $ΔHf° = -212.597 + 1.113\text{x}10^{-3}T + 2.574\text{x}10^{-6}T^{2} - 37.900T^{-1}$
$ΔGf° = -212.597 - 1.113\text{x}10^{-3}T\ln T - 2.574\text{x}10^{-6}T^{2} - 18.950T^{-1} + 49.710\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Weigel (517). Other data are those estimated by Oetting (356).

$PuOCl(c)$
Plutonium Oxychloride
[Formation: $Pu(c,l) + 0.5O_2(g) + 0.5Cl_2(g) = PuOCl(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.990	26.000	26.000	0	-221.100	-209.601	153.640
300	20.000	26.124	26.001	.037	-221.092	-209.530	152.641
395	20.542	31.696	26.729	1.962	-220.704	-205.927	113.936
395	20.542	31.696	26.729	1.962	-221.524	-205.927	113.936
400	20.570	31.955	26.792	2.065	-221.501	-205.730	112.404
480	21.026	35.745	27.976	3.729	-221.135	-202.609	92.249
480	21.026	35.745	27.976	3.729	-221.270	-202.609	92.249
500	21.140	36.606	28.304	4.151	-221.178	-201.834	88.220
588	21.650	40.074	29.812	6.034	-220.787	-198.463	73.764
588	21.650	40.074	29.812	6.034	-220.927	-198.463	73.764
600	21.720	40.512	30.022	6.294	-220.871	-198.004	72.122
700	22.290	43.903	31.769	8.494	-220.387	-194.232	60.641
730	22.461	44.842	32.287	9.165	-220.233	-193.114	57.814
730	22.461	44.842	32.287	9.165	-220.253	-193.114	57.814
752	22.586	45.511	32.664	9.661	-220.130	-192.298	55.886
752	22.586	45.511	32.664	9.661	-220.570	-192.298	55.886
800	22.860	46.917	33.477	10.752	-220.280	-190.503	52.042
900	23.430	49.642	35.124	13.066	-219.641	-186.819	45.365
913	23.504	49.979	35.333	13.371	-219.554	-186.345	44.606
913	23.504	49.979	35.333	13.371	-220.229	-186.345	44.606
1000	24.000	52.140	36.702	15.438	-219.790	-183.136	40.024
1100	24.570	54.454	38.212	17.866	-219.240	-179.497	35.662
1200	25.140	56.617	39.657	20.352	-218.637	-175.910	32.037
1300	25.710	58.652	41.041	22.894	-217.985	-172.377	28.979
1400	26.280	60.578	42.368	25.494	-217.279	-168.894	26.365
1500	26.860	62.411	43.644	28.151	-216.520	-165.464	24.108

*Data except enthalpy of formation at 298 K estimated.

<u>Phase changes</u>:
395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

<u>Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations</u>:

298.15-1500 K: $Cp° = 18.293 + 5.706\times10^{-3}T$
$H° - H°_{298} = 18.293\times10^{-3}T + 2.853\times10^{-6}T^2 - 5.708$

<u>Formation equations (kcal/mol)</u>:

298.15-395 K: $\Delta Hf° = -222.432 + 6.274\times10^{-3}T - 3.916\times10^{-6}T^2 - 56.750T^{-1}$
$\Delta Gf° = -222.432 - 6.274\times10^{-3}T\ln T + 3.916\times10^{-6}T^2 - 28.375T^{-1} + 77.937\times10^{-3}T$
395-480 K: $\Delta Hf° = -223.043 + 4.207\times10^{-3}T - 0.026\times10^{-6}T^2 - 56.750T^{-1}$
$\Delta Gf° = -223.043 - 4.207\times10^{-3}T\ln T + 0.026\times10^{-6}T^2 - 28.375T^{-1} + 68.661\times10^{-3}T$
480-588 K: $\Delta Hf° = -223.438 + 5.162\times10^{-3}T - 0.884\times10^{-6}T^2 - 56.750T^{-1}$
$\Delta Gf° = -223.438 - 5.162\times10^{-3}T\ln T + 0.884\times10^{-6}T^2 - 28.375T^{-1} + 74.969\times10^{-3}T$
588-730 K: $\Delta Hf° = -222.549 + 1.387\times10^{-3}T + 2.558\times10^{-6}T^2 - 56.750T^{-1}$
$\Delta Gf° = -222.549 - 1.387\times10^{-3}T\ln T - 2.558\times10^{-6}T^2 - 28.375T^{-1} + 51.408\times10^{-3}T$
730-752 K: $\Delta Hf° = -222.844 + 1.764\times10^{-3}T + 2.558\times10^{-6}T^2 - 56.750T^{-1}$
$\Delta Gf° = -222.844 - 1.764\times10^{-3}T\ln T - 2.558\times10^{-6}T^2 - 28.375T^{-1} + 54.298\times10^{-3}T$
752-913 K: $\Delta Hf° = -223.486 + 2.032\times10^{-3}T + 2.558\times10^{-6}T^2 - 56.750T^{-1}$
$\Delta Gf° = -223.486 - 2.032\times10^{-3}T\ln T - 2.558\times10^{-6}T^2 - 28.375T^{-1} + 56.926\times10^{-3}T$
913-1500 K: $\Delta Hf° = -222.455 + 0.164\times10^{-3}T + 2.558\times10^{-6}T^2 - 56.750T^{-1}$
$\Delta Gf° = -222.455 - 0.164\times10^{-3}T\ln T - 2.558\times10^{-6}T^2 - 28.375T^{-1} + 43.064\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Weigel (<u>518</u>). Other data are those estimated by Oetting (<u>356</u>).

$PuOF(c)$
Plutonium Oxyfluoride
[Formation: $Pu(c,l) + 0.5O_2(g) + 0.5F_2(g) = PuOF(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	18.990	21.900	21.900	0	-269.800	-257.801	188.971
300	19.000	22.017	21.900	.035	-269.793	-257.727	187.752
395	19.542	27.316	22.591	1.866	-269.470	-253.954	140.509
395	19.542	27.316	22.591	1.866	-270.290	-253.954	140.509
400	19.570	27.562	22.652	1.964	-270.271	-253.748	138.640
480	20.026	31.169	23.779	3.547	-269.966	-250.472	114.041
480	20.026	31.169	23.779	3.547	-270.101	-250.472	114.041
500	20.140	31.989	24.091	3.949	-270.024	-249.656	109.123
588	20.650	35.295	25.527	5.744	-269.704	-246.099	91.470
588	20.650	35.295	25.527	5.744	-269.844	-246.099	91.470
600	20.720	35.713	25.726	5.992	-269.798	-245.614	89.464
700	21.290	38.950	27.389	8.093	-269.398	-241.614	75.434
730	21.461	39.847	27.882	8.734	-269.270	-240.426	71.979
730	21.461	39.847	27.882	8.734	-269.290	-240.426	71.979
752	21.586	40.489	28.241	9.210	-269.184	-239.558	69.621
752	21.586	40.489	28.241	9.210	-269.624	-239.558	69.621
800	21.860	41.833	29.017	10.253	-269.377	-237.647	64.921
900	22.130	44.418	30.588	12.447	-268.849	-233.713	56.753
913	22.243	44.736	30.787	12.735	-268.777	-233.206	55.823
913	22.243	44.736	30.787	12.735	-269.452	-233.206	55.823
1000	23.000	46.797	32.091	14.706	-269.103	-229.767	50.215
1100	23.570	49.016	33.530	17.035	-268.646	-225.855	44.873
1200	21.140	51.091	34.908	19.420	-268.141	-221.987	40.429
1300	24.710	53.046	36.228	21.863	-267.583	-218.163	36.676
1400	25.280	54.898	37.497	24.362	-266.977	-214.385	33.467
1500	25.860	56.662	38.716	26.919	-266.316	-210.651	30.691

*Data estimated.

Phase changes:
395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 17.219 + 5.748\times10^{-3}T + 0.051\times10^{5}T^{-2}$
$H°-H°_{298} = 17.219\times10^{-3}T + 2.874\times10^{-6}T^{2} - 0.051\times10^{2}T^{-1} - 5.372$

Formation equations (kcal/mol):

298.15-395 K: $ΔHf° = -270.787 + 5.360\times10^{-3}T - 3.938\times10^{-6}T^{2} - 77.950T^{-1}$
$ΔGf° = -270.787 - 5.360\times10^{-3}T\ln T + 3.938\times10^{-6}T^{2} - 38.975T^{-1} + 73.356\times10^{-3}T$
395-480 K: $ΔHf° = -271.397 + 3.293\times10^{-3}T - 0.048\times10^{-6}T^{2} - 77.950T^{-1}$
$ΔGf° = -271.397 - 3.293\times10^{-3}T\ln T + 0.048\times10^{-6}T^{2} - 38.975T^{-1} + 64.080\times10^{-3}T$
480-588 K: $ΔHf° = -271.793 + 4.248\times10^{-3}T - 0.906\times10^{-6}T^{2} - 77.950T^{-1}$
$ΔGf° = -271.793 - 4.248\times10^{-3}T\ln T + 0.906\times10^{-6}T^{2} - 38.975T^{-1} + 70.388\times10^{-3}T$
588-730 K: $ΔHf° = -270.903 + 0.473\times10^{-3}T + 2.536\times10^{-6}T^{2} - 77.950T^{-1}$
$ΔGf° = -270.903 - 0.473\times10^{-3}T\ln T - 2.536\times10^{-6}T^{2} - 38.975T^{-1} + 46.827\times10^{-3}T$
730-752 K: $ΔHf° = -271.198 + 0.850\times10^{-3}T + 2.536\times10^{-6}T^{2} - 77.950T^{-1}$
$ΔGf° = -271.198 - 0.850\times10^{-3}T\ln T - 2.536\times10^{-6}T^{2} - 38.975T^{-1} + 49.717\times10^{-3}T$
752-913 K: $ΔHf° = -271.840 + 1.118\times10^{-3}T + 2.536\times10^{-6}T^{2} - 77.950T^{-1}$
$ΔGf° = -271.840 - 1.118\times10^{-3}T\ln T - 2.536\times10^{-6}T^{2} - 38.975T^{-1} + 52.345\times10^{-3}T$
913-1500 K: $ΔHf° = -270.809 - 0.750\times10^{-3}T + 2.536\times10^{-6}T^{2} - 77.950T^{-1}$
$ΔGf° = -270.809 + 0.750\times10^{-3}T\ln T - 2.536\times10^{-6}T^{2} - 38.975T^{-1} + 38.483\times10^{-3}T$

Source: Data are those estimated by Oetting (356).

PuOI(c)
Plutonium Oxyiodide
[Formation: $Pu(c,l) + 0.5O_2(g) + 0.5I_2(c,l,g) = PuOI(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	21.990	30.200	30.200	0	-197.800	-191.360	140.268
300	22.000	30.336	30.200	.041	-197.792	-191.319	139.374
386.8	22.495	35.987	30.890	1.972	-197.504	-189.488	107.063
386.8	22.495	35.987	30.890	1.972	-199.359	-189.488	107.063
395	22.542	36.459	31.000	2.156	-199.358	-189.279	104.725
395	22.542	36.459	31.000	2.156	-200.178	-189.279	104.725
400	22.570	36.743	31.070	2.269	-200.173	-189.142	103.341
458.4	22.903	39.841	31.994	3.597	-200.101	-187.534	89.409
458.4	22.903	39.841	31.994	3.597	-205.112	-187.534	89.409
480	23.026	40.899	32.371	4.093	-204.975	-186.708	85.009
480	23.026	40.899	32.371	4.093	-205.110	-186.708	85.009
500	23.140	41.841	32.731	4.555	-204.982	-185.945	81.275
588	23.650	45.632	34.385	6.614	-204.427	-182.641	67.884
588	23.650	45.632	34.385	6.614	-204.567	-182.641	67.884
600	23.720	46.111	34.614	6.898	-204.489	-182.194	66.363
700	24.290	49.810	36.527	9.298	-203.816	-178.530	55.739
730	24.461	50.833	37.094	10.029	-203.604	-177.451	53.125
730	24.461	50.833	37.094	10.029	-203.624	-177.451	53.125
752	24.586	51.561	37.506	10.569	-203.458	-176.665	51.342
752	24.586	51.561	37.506	10.569	-203.898	-176.665	51.342
800	24.860	53.091	38.396	11.756	-203.516	-174.939	47.790
900	25.430	56.052	40.196	14.270	-202.684	-171.417	41.625
913	25.504	56.417	40.425	14.601	-202.572	-170.967	40.925
913	25.504	56.417	40.425	14.601	-203.247	-170.967	40.925
1000	26.000	58.761	41.919	16.842	-202.638	-167.917	36.698
1100	26.570	61.265	43.565	19.470	-201.893	-164.480	32.679
1200	27.140	63.602	45.139	22.156	-201.096	-161.114	29.342
1300	27.710	65.797	46.645	24.898	-200.246	-157.817	26.531
1400	28.280	67.871	48.087	27.698	-199.344	-154.585	24.132
1500	28.850	69.842	49.473	30.554	-198.389	-151.423	22.062

*Data estimated.

Phase changes:
386.8 K, melting point of I_2 $\Delta H^\circ = 3.709$ kcal/mol.
395 K, α - β transition point of Pu; $\Delta H^\circ = 0.820$ kcal/mol.
458.4 K, boiling point of I_2 $\Delta H^\circ = 10.021$ kcal/mol.
480 K, β - γ transition point of Pu; $\Delta H^\circ = 0.135$ kcal/mol.
588 K, γ - δ transition point of Pu; $\Delta H^\circ = 0.140$ kcal/mol.
730 K, δ - δ' transition point of Pu; $\Delta H^\circ = 0.020$ kcal/mol.
752 K, δ' - ε transition point of Pu; $\Delta H^\circ = 0.440$ kcal/mol.
913 K, melting point of Pu; $\Delta H^\circ = 0.675$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 20.295 + 5.704\times10^{-3}T - 0.005\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 20.295\times10^{-3}T + 2.852\times10^{-6}T^2 + 0.005\times10^{2}T^{-1} - 6.306$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -199.179 + 6.251\times10^{-3}T - 4.619\times10^{-6}T^2 - 22.100T^{-1}$
$\Delta Gf^\circ = -199.179 - 6.251\times10^{-3}T\ln T + 4.619\times10^{-6}T^2 - 11.050T^{-1} + 60.593\times10^{-3}T$
386.8-395 K: $\Delta Hf^\circ = -199.907 + 3.049\times10^{-3}T - 3.873\times10^{-6}T^2 - 22.100T^{-1}$
$\Delta Gf^\circ = -199.907 - 3.049\times10^{-3}T\ln T + 3.873\times10^{-6}T^2 - 11.050T^{-1} + 43.685\times10^{-3}T$
395-458.4 K: $\Delta Hf^\circ = -200.517 + 0.982\times10^{-3}T + 0.017\times10^{-6}T^2 - 22.100T^{-1}$
$\Delta Gf^\circ = -200.517 - 0.982\times10^{-3}T\ln T - 0.017\times10^{-6}T^2 - 11.050T^{-1} + 34.409\times10^{-3}T$
458.4-480 K: $\Delta Hf^\circ = -207.874 + 6.152\times10^{-3}T - 0.018\times10^{-6}T^2 - 29.750T^{-1}$
$\Delta Gf^\circ = -207.874 - 6.152\times10^{-3}T\ln T + 0.018\times10^{-6}T^2 - 14.875T^{-1} + 82.140\times10^{-3}T$
480-588 K: $\Delta Hf^\circ = -208.270 + 7.107\times10^{-3}T - 0.876\times10^{-6}T^2 - 29.750T^{-1}$
$\Delta Gf^\circ = -208.270 - 7.107\times10^{-3}T\ln T + 0.876\times10^{-6}T^2 - 14.875T^{-1} + 88.449\times10^{-3}T$
588-730 K: $\Delta Hf^\circ = -207.380 + 3.332\times10^{-3}T + 2.567\times10^{-6}T^2 - 29.750T^{-1}$
$\Delta Gf^\circ = -207.380 - 3.332\times10^{-3}T\ln T - 2.567\times10^{-6}T^2 - 14.875T^{-1} + 64.888\times10^{-3}T$
730-752 K: $\Delta Hf^\circ = -207.675 + 3.709\times10^{-3}T + 2.567\times10^{-6}T^2 - 29.750T^{-1}$
$\Delta Gf^\circ = -207.675 - 3.709\times10^{-3}T\ln T - 2.567\times10^{-6}T^2 - 14.875T^{-1} + 67.778\times10^{-3}T$
752-913 K: $\Delta Hf^\circ = -208.317 + 3.977\times10^{-3}T + 2.567\times10^{-6}T^2 - 29.750T^{-1}$
$\Delta Gf^\circ = -208.317 - 3.977\times10^{-3}T\ln T - 2.567\times10^{-6}T^2 - 14.875T^{-1} + 70.406\times10^{-3}T$
913-1500 K: $\Delta Hf^\circ = -207.286 + 2.109\times10^{-3}T + 2.567\times10^{-6}T^2 - 29.750T^{-1}$
$\Delta Gf^\circ = -207.286 - 2.109\times10^{-3}T\ln T - 2.567\times10^{-6}T^2 - 14.875T^{-1} + 56.543\times10^{-3}T$

Source: Data are those estimated by Oetting (356).

$Pu(SO_4)_2(c)$
Plutonium Sulfate
[Reaction: $Pu(c,l) + S_2(g) + 4O_2(g) = Pu(SO_4)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15*	43.490	44.000	44.000	0	-565.710	-500.133	366.603
300	43.560	44.269	44.000	.081	-565.710	-499.725	364.045
395	48.804	56.941	45.629	4.468	-565.582	-478.842	264.935
395	48.804	56.941	45.629	4.468	-566.402	-478.842	264.935
400	49.080	57.557	45.774	4.713	-566.383	-477.734	261.018
480	53.496	66.896	48.529	8.816	-565.937	-460.039	209.459
480	53.496	66.896	48.529	8.816	-566.072	-460.039	209.459
500	54.600	69.102	49.308	9.897	-565.921	-455.625	199.151
588	59.458	78.336	52.970	14.916	-565.078	-436.279	162.156
588	59.458	78.336	52.970	14.916	-565.218	-436.279	162.156
600	60.120	79.544	53.489	15.633	-565.077	-433.648	157.954
700	65.640	89.235	57.912	21.926	-563.645	-411.851	128.584
730	67.098	92.020	59.257	23.917	-563.130	-405.356	121.355
730	67.098	92.020	59.257	23.917	-563.150	-405.356	121.355
752	68.167	94.029	60.243	25.407	-562.741	-400.608	116.425
752	68.167	94.029	60.243	25.407	-563.181	-400.608	116.425
800	70.500	98.319	62.400	28.735	-562.208	-390.262	106.613
900	75.150	106.894	66.873	36.019	-559.883	-368.906	89.581
913	75.722	107.976	67.450	37.000	-559.552	-366.150	87.646
913	75.722	107.976	67.450	37.000	-560.227	-366.150	87.646
1000	79.550	115.040	71.285	43.755	-558.002	-347.755	76.001
1100	83.860	122.826	75.620	51.927	-555.091	-326.867	64.942
1200	88.020	130.306	79.867	60.527	-551.795	-306.261	55.777
1300	91.480	137.490	84.025	69.505	-548.160	-285.946	48.071
1400	94.600	144.385	88.092	78.810	-544.238	-265.922	41.512
1500	97.550	151.013	92.067	88.419	-540.043	-246.189	35.869

*Data estimated.

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 33.618 + 45.578\times10^{-3}T - 3.304\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 33.618\times10^{-3}T + 22.789\times10^{-6}T^2 + 3.304\times10^{2}T^{-1} - 13.157$

Reaction equations (kcal/mol):

298.15-395 K: $\Delta Hr^\circ = -564.949 - 7.635\times10^{-3}T + 13.983\times10^{-6}T^2 + 81.300T^{-1}$
$\Delta Gr^\circ = -564.949 + 7.635\times10^{-3}T\ln T - 13.983\times10^{-6}T^2 + 40.650T^{-1} + 177.605\times10^{-3}T$
395-480 K: $\Delta Hr^\circ = -565.560 - 9.702\times10^{-3}T + 17.873\times10^{-6}T^2 + 81.300T^{-1}$
$\Delta Gr^\circ = -565.560 + 9.702\times10^{-3}T\ln T - 17.873\times10^{-6}T^2 + 40.650T^{-1} + 168.329\times10^{-3}T$
480-588 K: $\Delta Hr^\circ = -565.956 - 8.747\times10^{-3}T + 17.015\times10^{-6}T^2 + 81.300T^{-1}$
$\Delta Gr^\circ = -565.956 + 8.747\times10^{-3}T\ln T - 17.015\times10^{-6}T^2 + 40.650T^{-1} + 174.638\times10^{-3}T$
588-730 K: $\Delta Hr^\circ = -565.066 - 12.522\times10^{-3}T + 20.457\times10^{-6}T^2 + 81.300T^{-1}$
$\Delta Gr^\circ = -565.066 + 12.522\times10^{-3}T\ln T - 20.457\times10^{-6}T^2 + 40.650T^{-1} + 151.077\times10^{-3}T$
730-752 K: $\Delta Hr^\circ = -565.361 - 12.145\times10^{-3}T + 20.457\times10^{-6}T^2 + 81.300T^{-1}$
$\Delta Gr^\circ = -565.361 + 12.145\times10^{-3}T\ln T - 20.457\times10^{-6}T^2 + 40.650T^{-1} + 153.967\times10^{-3}T$
752-913 K: $\Delta Hr^\circ = -566.003 - 11.877\times10^{-3}T + 20.457\times10^{-6}T^2 + 81.300T^{-1}$
$\Delta Gr^\circ = -566.003 + 11.877\times10^{-3}T\ln T - 20.457\times10^{-6}T^2 + 40.650T^{-1} + 156.594\times10^{-3}T$
913-1500 K: $\Delta Hr^\circ = -564.972 - 13.745\times10^{-3}T + 20.457\times10^{-6}T^2 + 81.300T^{-1}$
$\Delta Gr^\circ = -564.972 + 13.745\times10^{-3}T\ln T - 20.457\times10^{-6}T^2 + 40.650T^{-1} + 142.732\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K are those estimated by Cordfunke (99). Other data are those estimated by Oetting (356).

$RbBF_4(c,l)$
Rubidium Tetrafluoroborate
[Formation: $Rb(c,l,g) + B(\beta) + 2F_2(g) = RbBF_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	27.800	39.000	39.000	0	-449.300	-426.150	312.372
300	27.870	39.170	39.003	.050	-449.297	-426.007	310.342
312.64	28.355	40.330	39.034	.405	-449.262	-425.026	297.109
312.64	28.355	40.330	39.034	.405	-449.786	-425.026	297.109
400	31.710	47.720	40.145	3.030	-449.494	-418.142	228.459
500	35.520	55.210	42.430	6.390	-448.917	-410.368	179.370
518	36.210	56.480	42.889	7.040	-448.778	-408.979	172.550
518	34.180	62.000	42.889	9.900	-445.918	-408.979	172.550
600	34.250	67.030	45.847	12.710	-445.469	-403.165	146.851
700	34.340	72.310	49.253	16.140	-444.968	-396.148	123.681
800	34.430	76.900	52.438	19.570	-444.507	-389.213	106.327
855	34.480	79.200	54.087	21.470	-444.253	-385.414	98.516
855	39.920	84.670	54.087	26.150	-439.573	-385.414	98.516
900	39.920	86.720	55.664	27.950	-439.128	-382.571	92.900
974.5	39.920	89.889	58.158	30.922	-438.418	-377.920	84.754
974.5	39.920	89.889	58.158	30.922	-455.648	-377.920	84.754
1000	39.920	90.920	58.980	31.940	-455.358	-375.890	82.150

*Entropy at 298 K estimated.

Phase changes: 312.64 K, melting point of Rb; ΔH° = 0.524 kcal/mol.
518 K, α - β transition point of $RbBF_4$; ΔH° = 2.860 kcal/mol.
855 K, melting point of $RbBF_4$; ΔH° = 4.680 kcal/mol.
974.5 K, boiling point of Rb to ideal monotomic gas; ΔH° = 17.230 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-518 K: $Cp° = 16.491 + 38.056\times10^{-3}T$
$H°-H°_{298} = 16.491\times10^{-3}T + 19.028\times10^{-6}T^2 - 6.608$
518-855 K: $Cp° = 33.721 + 0.890\times10^{-3}T$
$H°-H°_{298} = 33.721\times10^{-3}T + 0.445\times10^{-6}T^2 - 7.687$
855-1000 K: $Cp° = 39.920$
$H°-H°_{298} = 39.920\times10^{-3}T - 7.982$

Formation equations (kcal/mol):

298.15-312.64 K: $\Delta Hf° = -446.731 - 5.781\times10^{-3}T + 6.432\times10^{-6}T^2 - 422.500T^{-1}$
$\Delta Gf° = -446.731 + 5.781\times10^{-3}T\ln T - 6.432\times10^{-6}T^2 - 211.250T^{-1} + 40.386\times10^{-3}T$
312.64-518 K: $\Delta Hf° = -446.386 - 13.121\times10^{-3}T + 18.626\times10^{-6}T^2 - 349.300T^{-1}$
$\Delta Gf° = -446.386 + 13.121\times10^{-3}T\ln T - 18.626\times10^{-6}T^2 - 174.650T^{-1} + 0.553\times10^{-3}T$
518-855 K: $\Delta Hf° = -447.465 + 4.109\times10^{-3}T + 0.043\times10^{-6}T^2 - 349.300T^{-1}$
$\Delta Gf° = -447.465 - 4.109\times10^{-3}T\ln T - 0.043\times10^{-6}T^2 - 174.650T^{-1} + 100.696\times10^{-3}T$
855-974.5 K: $\Delta Hf° = -447.760 + 10.308\times10^{-3}T - 0.402\times10^{-6}T^2 - 349.300T^{-1}$
$\Delta Gf° = -447.760 - 10.308\times10^{-3}T\ln T + 0.402\times10^{-6}T^2 - 174.650T^{-1} + 142.511\times10^{-3}T$
974.5-1000 K: $\Delta Hf° = -467.102 + 13.191\times10^{-3}T - 1.038\times10^{-6}T^2 - 440.400T^{-1}$
$\Delta Gf° = -467.102 - 13.191\times10^{-3}T\ln T + 1.038\times10^{-6}T^2 - 220.200T^{-1} + 181.628\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Entropy at 298 K estimated. Other data based on Dworkin (133).

$Rb_2CO_3(c)$
Rubidium Carbonate
[Formation: $2Rb(c,l,g) + C(gr) + 1.5O_2(g) = Rb_2CO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.110	43.340	43.340	0	-273.500	-253.154	185.565
300	28.220	43.510	43.340	.052	-273.500	-253.027	184.328
312.64	28.731	44.685	43.368	.412	-273.491	-252.165	176.272
312.64	28.731	44.685	43.368	.412	-274.539	-252.165	176.272
400	32.260	52.250	44.507	3.097	-274.408	-245.923	134.365
500	34.720	59.720	46.814	6.453	-274.001	-238.846	104.398
600	36.580	66.230	49.527	10.022	-273.415	-231.871	84.458
700	38.140	71.980	52.324	13.759	-272.699	-224.996	70.246
800	39.540	77.170	55.115	17.644	-271.868	-218.240	59.620
900	40.860	81.900	57.828	21.665	-270.936	-211.576	51.377
974.5	41.799	85.186	59.794	24.745	-270.184	-206.698	46.355
974.5	41.799	85.186	59.794	24.745	-304.644	-206.698	46.355
1000	42.120	86.270	60.455	25.815	-304.277	-204.141	44.614
1100	43.340	90.350	62.997	30.088	-302.780	-194.196	38.583

Phase changes: 312.64 K, melting point of Rb; ΔH° = 0.524 kcal/mol.
974.5 K, boiling point of Rb to ideal monatomic gas; ΔH° = 17.230 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 31.532 + 11.190x10^{-3}T - 6.003x10^{5}T^{-2}$
$H°- H°_{298} = 31.532x10^{-3}T + 5.595x10^{-6}T^{2} + 6.003x10^{2}T^{-1} - 11.912$

Formation equations (kcal/mol):

298.15-312.64 K: $ΔHf° = -277.817 + 16.103x10^{-3}T - 19.038x10^{-6}T^{2} + 360.200T^{-1}$
$ΔGf° = -277.817 - 16.103x10^{-3}TlnT + 19.038x10^{-6}T^{2} + 180.100T^{-1} + 166.765x10^{-3}T$
312.64-974.5 K: $ΔHf° = -277.127 + 1.423x10^{-3}T + 5.351x10^{-6}T^{2} + 506.600T^{-1}$
$ΔGf° = -277.127 - 1.423x10^{-3}TlnT - 5.351x10^{-6}T^{2} + 253.300T^{-1} + 87.098x10^{-3}T$
974.5-1100 K: $ΔHf° = -315.811 + 7.189x10^{-3}T + 4.078x10^{-6}T^{2} + 324.400T^{-1}$
$ΔGf° = -315.811 - 7.189x10^{-3}TlnT - 4.078x10^{-6}T^{2} + 162.200T^{-1} + 165.332x10^{-3}T$

Source: Data from Chang (74).

Rb_2CrO_4(c,l)
Rubidium Chromate

[Formation: $2Rb(c,l,g) + Cr(c) + 2O_2(g) = Rb_2CrO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	34.895	51.530	51.530	0	-337.180	-310.695	227.743
300	34.928	51.745	51.530	.065	-337.179	-310.531	226.219
311.5	35.266	53.065	51.561	.469	-337.178	-309.509	217.150
312.64	35.299	53.194	51.567	.509	-337.181	-309.408	216.288
312.64	35.299	53.194	51.567	.509	-338.229	-309.408	216.288
400	37.866	62.161	52.929	3.693	-338.196	-301.352	164.649
500	41.085	70.968	55.676	7.646	-337.863	-292.175	127.708
600	43.210	78.666	58.884	11.869	-337.282	-283.090	103.114
700	44.560	85.430	62.201	16.260	-336.564	-274.110	85.580
800	47.170	91.279	65.252	20.822	-335.708	-265.054	72.409
900	54.766	97.440	68.709	25.858	-334.410	-256.493	62.284
974.5	68.084	102.206	71.085	30.327	-332.759	-250.115	56.092
974.5	68.084	102.206	71.085	30.327	-367.219	-250.115	56.092
998	72.285	103.878	71.838	31.976	-366.373	-247.303	54.156
998	46.142	105.191	71.838	33.286	-365.063	-247.303	54.156
1000	46.288	105.284	71.904	33.380	-365.038	-247.066	53.996
1100	53.552	110.036	75.152	38.372	-363.504	-235.334	46.756
1200	60.817	115.007	78.266	44.089	-361.301	-223.773	40.754
1261	65.251	118.130	80.118	47.934	-359.630	-216.827	37.579
1261	51.245	124.094	80.118	55.454	-352.110	-216.827	37.579
1300	51.245	125.719	81.525	57.452	-351.513	-212.737	35.764
1400	51.245	129.453	84.756	62.576	-350.020	-202.036	31.539
1500	51.245	132.988	87.854	67.701	-348.575	-191.504	27.902

Phase changes: 311.5 K, second-order transition point of Cr; ΔH° = 0 kcal/mol.
312.64 K, melting point of Rb; ΔH° = 0.524 kcal/mol.
974.5 K, boiling point of Rb to ideal monotomic gas; ΔH° = 17.230 kcal/mol.
998 K, α - β transition point of Rb_2CrO_4; ΔH° = 1.310 kcal/mol.
1261 K, melting point of Rb_2CrO_4; ΔH° = 7.520 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-998 K: $Cp^\circ = 19.822 + 38.220\times10^{-3}T + 3.268\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 19.822\times10^{-3}T + 19.110\times10^{-6}T^2 - 3.268\times10^{2}T^{-1} - 6.513$
998-1261 K: $Cp^\circ = -26.369 + 72.656\times10^{-3}T$
$H^\circ - H^\circ_{298} = -26.369\times10^{-3}T + 36.328\times10^{-6}T^2 + 23.419$
1261-1500 K: $Cp^\circ = 51.245$
$H^\circ - H^\circ_{298} = 51.245\times10^{-3}T - 9.166$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -336.203 + 7.104\times10^{-3}T - 19.075\times10^{-6}T^2 - 417.200T^{-1}$
$\Delta Gf^\circ = -336.203 - 7.104\times10^{-3}T\ln T + 19.075\times10^{-6}T^2 - 208.600T^{-1} + 122.689\times10^{-3}T$
311.5-312.64 K: $\Delta Hf^\circ = -335.205 - 0.063\times10^{-3}T - 6.799\times10^{-6}T^2 - 403.600T^{-1}$
$\Delta Gf^\circ = -335.205 + 0.063\times10^{-3}T\ln T + 6.799\times10^{-6}T^2 - 201.800T^{-1} + 82.091\times10^{-3}T$
312.64-974.5 K: $\Delta Hf^\circ = -334.516 - 14.743\times10^{-3}T + 17.589\times10^{-6}T^2 - 257.200T^{-1}$
$\Delta Gf^\circ = -334.516 + 14.743\times10^{-3}T\ln T - 17.589\times10^{-6}T^2 - 128.600T^{-1} + 2.424\times10^{-3}T$
974.5-998 K: $\Delta Hf^\circ = -373.200 - 8.977\times10^{-3}T + 16.317\times10^{-6}T^2 - 439.400T^{-1}$
$\Delta Gf^\circ = -373.200 + 8.977\times10^{-3}T\ln T - 16.317\times10^{-6}T^2 - 219.700T^{-1} + 80.658\times10^{-3}T$
998-1261 K: $\Delta Hf^\circ = -343.268 - 55.168\times10^{-3}T + 33.535\times10^{-6}T^2 - 112.600T^{-1}$
$\Delta Gf^\circ = -343.268 + 55.168\times10^{-3}T\ln T - 33.535\times10^{-6}T^2 - 56.300T^{-1} - 251.298\times10^{-3}T$
1261-1500 K: $\Delta Hf^\circ = -375.853 + 22.446\times10^{-3}T - 2.793\times10^{-6}T^2 - 112.600T^{-1}$
$\Delta Gf^\circ = -375.853 - 22.446\times10^{-3}T\ln T + 2.793\times10^{-6}T^2 - 56.300T^{-1} + 282.871\times10^{-3}T$

Source: Data from O'Hare (370).

$RbPO_3(c)$
Rubidium Metaphosphate
[Formation: $Rb(c,l) + P(c,l,1/4P_4(g)) + 1.5O_2(g) = RbPO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	24.430	27.230	27.230	0	-295.700	-273.503	200.481
300	24.460	27.380	27.230	.050	-295.695	-273.361	199.141
312.64	24.661	28.394	27.241	.360	-295.685	-272.419	190.431
312.64	24.661	28.394	27.241	.360	-296.209	-272.419	190.431
317.3	24.735	28.759	27.260	.476	-296.209	-272.065	187.390
317.3	24.735	28.759	27.260	.476	-296.366	-272.065	187.390
400	26.050	34.640	28.215	2.570	-296.337	-265.739	145.191
500	27.640	40.620	30.120	5.250	-296.151	-258.112	112.819
550	28.430	43.292	31.185	6.659	-295.990	-254.323	101.057
550	28.430	43.292	31.185	6.659	-298.898	-254.323	101.057
600	29.220	45.800	32.300	8.100	-298.626	-250.282	91.164
700	30.810	50.420	34.563	11.100	-297.980	-242.272	75.640

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 312.64 K, melting point of Rb; ΔH° = 0.524 kcal/mol.
317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol. of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 19.700 + 15.870\times10^{-3}T$
$H°-H°_{298} = 19.700\times10^{-3}T + 7.935\times10^{-6}T^2 - 6.579$

Formation equations (kcal/mol):

298.15-312.64 K: $\Delta Hf° = -296.149 + 4.523\times10^{-3}T - 7.561\times10^{-6}T^2 - 67.800T^{-1}$
$\Delta Gf° = -296.149 - 4.523\times10^{-3}T\ln T + 7.561\times10^{-6}T^2 - 33.900T^{-1} + 99.851\times10^{-3}T$
312.64-317.3 K: $\Delta Hf° = -295.804 - 2.817\times10^{-3}T + 4.633\times10^{-6}T^2 + 5.400T^{-1}$
$\Delta Gf° = -295.804 + 2.817\times10^{-3}T\ln T - 4.633\times10^{-6}T^2 + 2.700T^{-1} + 60.017\times10^{-3}T$
317.3-550 K: $\Delta Hf° = -295.491 - 5.310\times10^{-3}T + 7.818\times10^{-6}T^2 + 5.400T^{-1}$
$\Delta Gf° = -295.491 + 5.310\times10^{-3}T\ln T - 7.818\times10^{-6}T^2 + 2.700T^{-1} + 45.681\times10^{-3}T$
550-700 K: $\Delta Hf° = -298.951 - 3.972\times10^{-3}T + 7.814\times10^{-6}T^2 - 94.900T^{-1}$
$\Delta Gf° = -298.951 + 3.972\times10^{-3}T\ln T - 7.814\times10^{-6}T^2 - 47.450T^{-1} + 60.579\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data are those estimated by Beglov (25).

$Rb_2SO_4(c,l)$
Rubidium Sulfate
[Reaction: $2Rb(c,l,g) + 0.5S_2(g) + 2O_2(g) = Rb_2SO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	32.011	47.190	47.190	0	-358.475	-324.255	237.683
300	32.087	47.388	47.191	.059	-358.477	-324.043	236.062
312.64	32.539	48.722	47.226	.467	-358.488	-322.592	225.504
312.64	32.539	48.722	47.226	.467	-359.536	-322.592	225.504
400	35.663	57.136	48.494	3.457	-359.542	-312.259	170.608
500	38.619	65.405	51.069	7.168	-359.242	-300.470	131.334
600	41.692	72.719	54.079	11.184	-358.635	-288.768	105.182
700	45.230	79.394	57.224	15.519	-357.716	-277.190	86.541
800	52.335	85.828	60.397	20.345	-356.319	-265.774	72.605
900	69.840	92.855	63.602	26.328	-353.784	-254.577	61.819
931	78.971	95.367	64.616	28.629	-352.558	-251.180	58.963
931	43.881	95.479	64.616	28.733	-352.454	-251.180	58.963
974.5	45.053	97.509	66.040	30.667	-352.035	-246.465	55.274
974.5	45.053	97.509	66.040	30.667	-386.495	-246.465	55.274
1000	45.740	98.682	66.857	31.825	-386.129	-242.806	53.065
1100	48.435	103.168	69.955	36.534	-384.539	-228.547	45.408
1200	51.129	107.498	72.905	41.512	-382.703	-214.446	39.056
1300	53.824	111.697	75.729	46.759	-380.614	-200.507	33.708
1339	54.874	113.303	76.799	48.879	-379.732	-195.116	31.846
1339	49.335	120.159	76.799	58.059	-370.552	-195.116	31.846
1400	49.335	122.357	78.736	61.069	-369.484	-187.148	29.215
1500	49.335	125.761	81.760	66.002	-367.748	-174.187	25.379
1600	49.335	128.945	84.611	70.935	-366.030	-161.340	22.038
1700	49.335	131.936	87.307	75.869	-364.326	-148.598	19.103
1800	49.335	134.755	89.865	80.802	-362.637	-135.953	16.507
1900	49.335	137.423	92.299	85.736	-360.966	-123.408	14.195
2000	49.335	139.953	94.619	90.669	-359.314	-110.949	12.124

Phase changes: 312.64 K, melting point of Rb; ΔH° = 0.524 kcal/mol.
931 K, α - β transition point of Rb_2SO_4; ΔH° = 0.104 kcal/mol.
974.5 K, boiling point of Rb to ideal monotomic gas; ΔH° = 17.230 kcal/mol.
1339 K, melting point of Rb_2SO_4; ΔH° = 9.180 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-931 K: $Cp° = -1.082 + 68.816\times10^{-3}T + 11.177\times10^{5}T^{-2}$
$H°-H°_{298} = -1.082\times10^{-3}T + 34.408\times10^{-6}T^{2} - 11.177\times10^{2}T^{-1} + 1.013$
931-1339 K: $Cp° = 18.940 + 26.854\times10^{-3}T - 0.518\times10^{5}T^{-2}$
$H°-H°_{298} = 18.940\times10^{-3}T + 13.427\times10^{-6}T^{2} + 0.518\times10^{2}T^{-1} - 0.594$
1339-2000 K: $Cp° = 49.335$
$H°-H°_{298} = 49.335\times10^{-3}T - 8.001$

Reaction equations (kcal/mol):

298.15-312.64 K: $\Delta Hr° = -349.014 - 20.779\times10^{-3}T + 10.130\times10^{-6}T^{2} - 1242.250T^{-1}$
$\Delta Gr° = -349.014 + 20.779\times10^{-3}T\ln T - 10.130\times10^{-6}T^{2} - 621.125T^{-1} - 25.347\times10^{-3}T$
312.64-931 K: $\Delta Hr° = -348.324 - 35.459\times10^{-3}T + 34.518\times10^{-6}T^{2} - 1095.850T^{-1}$
$\Delta Gr° = -348.324 + 35.459\times10^{-3}T\ln T - 34.518\times10^{-6}T^{2} - 547.925T^{-1} - 105.014\times10^{-3}T$
931-974.5 K: $\Delta Hr° = -349.931 - 15.438\times10^{-3}T + 13.537\times10^{-6}T^{2} + 73.650T^{-1}$
$\Delta Gr° = -349.931 + 15.438\times10^{-3}T\ln T - 13.537\times10^{-6}T^{2} + 36.825T^{-1} + 13.380\times10^{-3}T$
974.5-1339 K: $\Delta Hr° = -388.615 - 9.672\times10^{-3}T + 12.265\times10^{-6}T^{2} - 108.550T^{-1}$
$\Delta Gr° = -388.615 + 9.672\times10^{-3}T\ln T - 12.265\times10^{-6}T^{2} - 54.275T^{-1} + 91.614\times10^{-3}T$
1339-2000 K: $\Delta Hr° = -396.022 + 20.723\times10^{-3}T - 1.162\times10^{-6}T^{2} - 160.350T^{-1}$
$\Delta Gr° = -396.022 - 20.723\times10^{-3}T\ln T + 1.162\times10^{-6}T^{2} - 80.175T^{-1} + 298.015\times10^{-3}T$

Source: Data from DeKock (113).

$Rb_2ZrO_3(c)$
Rubidium Zirconate
[Formation: $2Rb(c,l) + Zr(c) + 1.5O_2(g) = Rb_2ZrO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	31.880	43.810	43.810	0	-413.600	-391.025	286.625
300	32.050	44.010	43.810	.060	-413.599	-390.884	284.755
312.64	32.702	45.346	43.845	.469	-413.593	-389.927	272.574
312.64	32.702	45.346	43.845	.469	-414.641	-389.927	272.574
400	37.210	54.010	45.135	3.550	-414.458	-383.033	209.277
500	40.420	62.680	47.800	7.440	-413.867	-375.243	164.017
600	42.870	70.270	50.920	11.610	-412.996	-367.593	133.894
700	44.950	77.040	54.183	16.000	-411.915	-360.112	112.431
800	46.840	83.170	57.432	20.590	-410.656	-352.800	96.379

*Enthalpy of formation and entropy at 298 K estimated.

Phase change: 312.64 K, melting point of Rb; ΔH° = 0.524 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 36.003 + 14.982 \times 10^{-3}T - 7.636 \times 10^{5}T^{-2}$
$H° - H°_{298} = 36.003 \times 10^{-3}T + 7.491 \times 10^{-6}T^{2} + 7.636 \times 10^{2}T^{-1} - 13.961$

Formation equations (kcal/mol):

298.15-312.64 K: $\Delta Hf° = -419.680 + 18.099 \times 10^{-3}T - 17.318 \times 10^{-6}T^{2} + 662.900T^{-1}$
$\Delta Gf° = -419.680 - 18.099 \times 10^{-3}T\ln T + 17.318 \times 10^{-6}T^{2} + 331.450T^{-1} + 190.340 \times 10^{-3}T$
312.64-800 K: $\Delta Hf° = -418.991 + 3.419 \times 10^{-3}T + 7.070 \times 10^{-6}T^{2} + 809.300T^{-1}$
$\Delta Gf° = -418.991 - 3.419 \times 10^{-3}T\ln T - 7.070 \times 10^{-6}T^{2} + 404.650T^{-1} + 110.672 \times 10^{-3}T$

Source: Data from Kohli (278) who estimated enthalpy of formation and entropy at 298 K.

ReO(g)
Rhenium Monoxide (ideal gas)
[Formation: Re(c) + $0.5O_2(g)$ = ReO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.480	58.061	58.061	0	95.000	87.597	-64.210
300	7.490	58.108	58.061	.014	94.996	87.552	-63.780
400	7.830	60.309	58.359	.780	94.796	85.101	-46.496
500	8.120	62.091	58.933	1.579	94.604	82.699	-36.147
600	8.320	63.589	59.587	2.401	94.410	80.336	-29.262
700	8.460	64.883	60.253	3.241	94.211	78.007	-24.355
800	8.560	66.020	60.905	4.092	94.000	75.705	-20.681
900	8.630	67.032	61.530	4.952	93.776	73.432	-17.832
1000	8.680	67.945	62.127	5.818	93.538	71.184	-15.557
1100	8.730	68.774	62.694	6.688	93.286	68.961	-13.701
1200	8.760	69.536	63.234	7.563	93.021	66.761	-12.159
1300	8.780	70.237	63.745	8.440	92.741	64.584	-10.857
1400	8.800	70.889	64.233	9.319	92.446	62.429	-9.745
1500	8.820	71.498	64.697	10.201	92.138	60.295	-8.785
1600	8.840	72.068	65.141	11.084	91.814	58.181	-7.947
1700	8.850	72.603	65.563	11.968	91.476	56.092	-7.211
1800	8.860	73.110	65.969	12.853	91.123	54.020	-6.559
1900	8.870	73.588	66.357	13.739	90.755	51.969	-5.978
2000	8.870	74.043	66.730	14.626	90.372	49.938	-5.457

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.357 + 0.346x10^{-3}T - 0.871x10^{5}T^{-2}$

$H°- H°_{298} = 8.357x10^{-3}T + 0.173x10^{-6}T^{2} + 0.871x10^{2}T^{-1} - 2.799$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 95.135 - 0.934x10^{-3}T - 0.725x10^{-6}T^{2} + 62.100T^{-1}$

$\Delta Gf° = 95.135 + 0.934x10^{-3}T\ln T + 0.725x10^{-6}T^{2} + 31.050T^{-1} - 31.167x10^{-3}T$

Source: Data from Pedley (396).

RhO(g)
Rhodium Monoxide (ideal gas)
[Formation: $Rh(c,l) + 0.5O_2(g) = RhO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.590	57.673	57.673	0	95.000	87.359	-64.035
300	7.600	57.720	57.673	.014	94.996	87.312	-63.606
400	7.980	59.961	57.976	.794	94.811	84.778	-46.320
500	8.240	61.772	58.560	1.606	94.618	82.292	-35.969
600	8.420	63.290	59.225	2.439	94.412	79.847	-29.084
700	8.540	64.598	59.901	3.288	94.187	77.437	-24.177
800	8.620	65.745	60.563	4.146	93.939	75.059	-20.505
900	8.680	66.764	61.195	5.012	93.671	72.715	-17.657
1000	8.730	67.682	61.799	5.883	93.380	70.402	-15.386
1100	8.760	68.515	62.372	6.757	93.066	68.120	-13.534
1200	8.790	69.279	62.917	7.635	92.728	65.867	-11.996
1300	8.810	69.984	63.433	8.516	92.366	63.643	-10.699
1400	8.830	70.638	63.925	9.398	91.976	61.448	-9.592
1500	8.840	71.247	64.393	10.281	91.557	59.281	-8.637
1600	8.850	71.818	64.839	11.166	91.108	57.144	-7.805
1700	8.860	72.355	65.266	12.052	90.627	55.036	-7.075
1800	8.870	72.862	65.674	12.939	90.110	52.958	-6.430
1900	8.880	73.342	66.065	13.827	89.553	50.908	-5.856
2000	8.890	73.799	66.442	14.715	88.954	48.888	-5.342
2100	8.890	74.231	66.801	15.604	88.307	46.903	-4.881
2200	8.900	74.646	67.149	16.493	87.610	44.944	-4.465
2237	8.900	74.794	67.274	16.822	87.338	44.230	-4.321
2237	8.900	74.794	67.274	16.822	80.982	44.230	-4.321
2300	8.900	75.041	67.483	17.383	80.492	43.202	-4.105
2400	8.900	75.420	67.806	18.273	79.713	41.596	-3.788
2500	8.910	75.783	68.118	19.163	78.931	40.026	-3.499

Phase change: 2237 K, melting point of Rh; ΔH° = 6.356 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 8.555 + 0.206\times10^{-3}T - 0.912\times10^{5}T^{-2}$

$H°-H°_{298} = 8.555\times10^{-3}T + 0.103\times10^{-6}T^{2} + 0.912\times10^{2}T^{-1} - 2.866$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 94.898 - 0.106\times10^{-3}T - 1.475\times10^{-6}T^{2} + 78.800T^{-1}$

$\Delta Gf° = 94.898 + 0.106\times10^{-3}T\ln T + 1.475\times10^{-6}T^{2} + 39.400T^{-1} - 26.775\times10^{-3}T$

2000-2237 K: $\Delta Hf° = 95.567 - 0.661\times10^{-3}T - 1.328\times10^{-6}T^{2} - 213.600T^{-1}$

$\Delta Gf° = 95.567 + 0.661\times10^{-3}T\ln T + 1.328\times10^{-6}T^{2} - 106.800T^{-1} - 30.997\times10^{-3}T$

2237-2500 K: $\Delta Hf° = 98.332 - 7.705\times10^{-3}T - 0.002\times10^{-6}T^{2} - 223.800T^{-1}$

$\Delta Gf° = 98.332 + 7.705\times10^{-3}T\ln T + 0.002\times10^{-6}T^{2} - 111.900T^{-1} - 83.593\times10^{-3}T$

Source: Data from Pedley (396).

$Ru(CO)_5(g)$
Ruthenium Pentacarbonyl (ideal gas)
[Formation: $Ru(c) + 5C(c) + 2.5O_2(g) = Ru(CO)_5(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	42.290	110.450	110.450	0	-252.000	-244.319	179.089
300	42.380	110.710	110.450	.078	-251.986	-244.272	177.950
400	46.250	123.480	112.163	4.527	-251.121	-241.829	132.128
500	48.770	134.090	115.520	9.285	-250.392	-239.597	104.726
600	50.720	143.160	119.388	14.263	-249.824	-237.489	86.504
700	52.320	151.100	123.361	19.417	-249.394	-235.471	73.516
800	53.660	158.180	127.282	24.718	-249.057	-233.509	63.791
900	54.770	164.560	131.070	30.141	-248.794	-231.581	56.235
1000	55.700	170.380	134.714	35.666	-248.577	-229.680	50.196

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 45.674 + 10.982x10^{-3}T - 5.919x10^{5}T^{-2}$
$H°- H°_{298} = 45.674x10^{-3}T + 5.491x10^{-6}T^{2} + 5.919x10^{2}T^{-1} - 16.091$

Formation equations (kcal/mol):

298.15-1000 K: $ΔHf° = -252.318 + 5.302x10^{-3}T - 0.800x10^{-6}T^{2} - 355.400T^{-1}$
$ΔGf° = -252.318 - 5.302x10^{-3}TlnT + 0.800x10^{-6}T^{2} - 177.700T^{-1} + 58.796x10^{-3}T$

Source: Data from Behrens (26).

$RuO(g)$
Ruthenium Monoxide (ideal gas)
[Formation: $Ru(c) + 0.5O_2(g) = RuO(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.540	57.851	57.851	0	89.000	81.096	-59.444
300	7.540	57.898	57.851	.014	88.996	81.047	-59.042
400	7.900	60.119	58.152	.787	88.826	78.423	-42.848
500	8.180	61.914	58.730	1.592	88.648	75.843	-33.150
600	8.370	63.423	59.390	2.420	88.460	73.300	-26.699
700	8.500	64.724	60.061	3.264	88.257	70.788	-22.101
800	8.590	65.866	60.717	4.119	88.039	68.307	-18.660
900	8.660	66.883	61.347	4.982	87.805	65.854	-15.991
1000	8.710	67.797	61.947	5.850	87.554	63.429	-13.862
1100	8.750	68.629	62.517	6.723	87.288	61.029	-12.125
1200	8.770	69.392	63.059	7.599	87.007	58.654	-10.682
1300	8.800	70.095	63.573	8.478	86.708	56.303	-9.465
1400	8.820	70.748	64.063	9.359	86.393	53.976	-8.426
1500	8.830	71.357	64.529	10.242	86.058	51.672	-7.528
1600	8.850	71.928	64.974	11.126	85.702	49.391	-6.746
1700	8.860	72.464	65.399	12.011	85.323	47.134	-6.059
1800	8.870	72.971	65.806	12.897	84.917	44.898	-5.451
1900	8.870	73.450	66.195	13.784	84.482	42.687	-4.910
2000	8.880	73.906	66.570	14.671	84.012	40.497	-4.425

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.442 + 0.290\times10^{-3}T - 0.878\times10^{5}T^{-2}$

$H°-H°_{298} = 8.442\times10^{-3}T + 0.145\times10^{-6}T^{2} + 0.878\times10^{2}T^{-1} - 2.824$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 88.771 + 0.120\times10^{-3}T - 1.311\times10^{-6}T^{2} + 92.400T^{-1}$

$\Delta Gf° = 88.771 - 0.120\times10^{-3}T\ln T + 1.311\times10^{-6}T^{2} + 46.200T^{-1} - 25.967\times10^{-3}T$

Source: Data from Pedley (396).

$RuSe_2(c)$
Ruthenium Diselenide
[Reaction: $Ru(c) + Se_2(g) = RuSe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	16.730	19.500	19.500	0	-71.900	-58.323	42.751
300	16.740	19.600	19.500	.030	-71.899	-58.239	42.426
400	17.500	24.530	20.155	1.750	-71.763	-53.700	29.340
500	17.990	28.490	21.450	3.520	-71.618	-49.206	21.508
600	18.370	31.810	22.910	5.340	-71.447	-44.743	16.297
700	18.710	34.660	24.389	7.190	-71.265	-40.304	12.583
800	19.020	37.180	25.830	9.080	-71.058	-35.889	9.804
900	19.320	39.440	27.218	11.000	-70.832	-31.507	7.651
1000	19.610	41.490	28.540	12.950	-70.586	-27.149	5.933
1100	19.890	43.380	29.816	14.920	-70.329	-22.829	4.536
1200	20.170	45.120	31.020	16.920	-70.051	-18.522	3.373

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 17.060 + 2.650\times10^{-3}T - 1.000\times10^{5}T^{-2}$

$H°-H°_{298} = 17.060\times10^{-3}T + 1.325\times10^{-6}T^{2} + 1.000\times10^{2}T^{-1} - 5.540$

Reaction equations (kcal/mol):

298.15-1200 K: $\Delta Hr° = -72.668 + 1.689\times10^{-3}T + 0.440\times10^{-6}T^{2} + 67.300T^{-1}$

$\Delta Gr° = -72.668 - 1.689\times10^{-3}T\ln T - 0.440\times10^{-6}T^{2} + 33.650T^{-1} + 57.492\times10^{-3}T$

Source: Data from Mills (332) who estimated all except enthalpy of formation at 298 K.

$RuTe_2(c)$
Ruthenium Ditelluride
[Reaction: $Ru(c) + Te_2(g) = RuTe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	17.700	21.400	21.400	0	-71.830	-57.725	42.313
300	17.720	21.510	21.400	.033	-71.824	-57.639	41.989
400	18.230	26.690	22.103	1.835	-71.490	-52.959	28.935
500	18.390	30.780	23.446	3.667	-71.171	-48.365	21.140
600	18.470	34.140	24.955	5.511	-70.878	-43.826	15.963
700	18.580	36.990	26.471	7.363	-70.613	-39.337	12.281
800	18.730	39.480	27.945	9.228	-70.369	-34.888	9.531
900	18.960	41.700	29.353	11.112	-70.136	-30.469	7.399
1000	19.250	43.720	30.698	13.022	-69.909	-26.082	5.700
1100	19.610	45.570	31.966	14.964	-69.679	-21.706	4.312
1200	20.050	47.290	33.167	16.947	-69.440	-17.347	3.159
1300	20.560	48.920	34.322	18.977	-69.184	-13.024	2.190
1400	21.140	50.460	35.416	21.061	-68.906	-8.710	1.360
1500	21.780	51.940	36.469	23.206	-68.588	-4.424	.645

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 17.167 + 2.334 \times 10^{-3}T - 0.145 \times 10^{5}T^{-2}$

$H°-H°_{298} = 17.167 \times 10^{-3}T + 1.167 \times 10^{-6}T^{2} + 0.145 \times 10^{2}T^{-1} - 5.271$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta Hr° = -72.984 + 3.861 \times 10^{-3}T - 0.630 \times 10^{-6}T^{2} + 17.500T^{-1}$

$\Delta Gr° = -72.984 - 3.861 \times 10^{-3}T\ln T + 0.630 \times 10^{-6}T^{2} + 8.750T^{-1} + 72.891 \times 10^{-3}T$

Source: Data from Svendsen (489).

Sb_2Se_3(c,l)
Diantimony Triselenide
[Reaction: $2Sb(c,l) + 1.5Se_2(g) = Sb_2Se_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15	29.870	50.700	50.700	0	-80.450	-63.050	46.216
300	29.880	50.880	50.713	.050	-80.449	-62.944	45.854
400	30.380	59.550	51.875	3.070	-80.146	-57.149	31.225
500	30.880	66.380	54.120	6.130	-79.852	-51.434	22.481
600	31.380	72.060	56.660	9.240	-79.538	-45.797	16.681
700	31.880	76.930	59.201	12.410	-79.201	-40.180	12.544
800	32.380	81.220	61.695	15.620	-78.875	-34.635	9.462
888	32.820	84.620	63.798	18.490	-78.594	-29.780	7.329
888	41.000	99.090	63.798	31.340	-65.744	-29.780	7.329
900	41.000	99.640	64.273	31.830	-65.611	-29.296	7.114
903.9	41.000	99.817	64.426	31.990	-65.568	-29.138	7.045
903.9	41.000	99.817	64.426	31.990	-75.068	-29.138	7.045
1000	41.000	103.960	68.030	35.930	-74.008	-24.323	5.316

Phase changes: 888 K, melting point of Sb_2Se_3; ΔH° = 12.880 kcal/mol.
903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-888 K: $Cp^\circ = 28.381 + 5.000\times10^{-3}T$
$H^\circ - H^\circ_{298} = 28.381\times10^{-3}T + 2.500\times10^{-6}T^2 - 8.684$
888-1000 K: $Cp^\circ = 41.000$
$H^\circ - H^\circ_{298} = 41.000\times10^{-3}T - 5.068$

Reaction equations (kcal/mol):

298.15-888 K: $\Delta Hr^\circ = -81.009 + 2.209\times10^{-3}T + 0.635\times10^{-6}T^2 - 46.650T^{-1}$
$\Delta Gr^\circ = -81.009 - 2.209\times10^{-3}T\ln T - 0.635\times10^{-6}T^2 - 23.325T^{-1} + 73.271\times10^{-3}T$
888-903.9 K: $\Delta Hr^\circ = -77.393 + 14.828\times10^{-3}T - 1.865\times10^{-6}T^2 - 46.650T^{-1}$
$\Delta Gr^\circ = -77.393 - 14.828\times10^{-3}T\ln T + 1.865\times10^{-6}T^2 - 23.325T^{-1} + 152.649\times10^{-3}T$
903.9-1000 K: $\Delta Hr^\circ = -84.400 + 10.004\times10^{-3}T + 0.479\times10^{-6}T^2 - 89.850T^{-1}$
$\Delta Gr^\circ = -84.400 - 10.004\times10^{-3}T\ln T - 0.479\times10^{-6}T^2 - 44.925T^{-1} + 129.711\times10^{-3}T$

Source: Data from Mills (332).

Sb_2Te_3(c,l)
Diantimony Tritelluride
[Reaction: $2Sb(c,l) + 1.5Te_2(g) = Sb_2Te_3(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	30.770	58.900	58.900	0	-70.995	-54.398	39.875
300*	30.790	59.090	58.900	.057	-70.984	-54.295	39.553
400	32.060	68.120	60.123	3.199	-70.385	-48.819	26.673
500	33.330	75.410	62.472	6.469	-69.713	-43.500	19.014
600	34.600	81.600	65.158	9.865	-68.966	-38.330	13.962
700	35.870	87.030	67.903	13.389	-68.154	-33.283	10.391
800	37.140	91.900	70.601	17.039	-67.295	-28.371	7.750
892	38.310	96.000	73.008	20.510	-66.471	-23.934	5.864
892	47.000	122.550	73.008	44.190	-42.791	-23.934	5.864
900	47.000	122.980	73.462	44.566	-42.649	-23.776	5.774
903.9	47.000	123.183	73.676	44.749	-42.580	-23.694	5.729
903.9	47.000	123.183	73.676	44.749	-52.080	-23.694	5.729
1000	47.000	127.930	78.664	49.266	-50.414	-20.769	4.539

*Data above 298 K estimated except temperature and enthalpy of fusion.

Phase changes: 888 K, melting point of Sb_2Te_3; ΔH° = 23.680 kcal/mol.
903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-892 K: $Cp° = 26.980 + 12.700\times10^{-3}T$
$H° - H°_{298} = 26.980\times10^{-3}T + 6.350\times10^{-6}T^2 - 8.609$
892-1000 K: $Cp° = 47.000$
$H° - H°_{298} = 47.000\times10^{-3}T + 2.266$

Reaction equations (kcal/mol):

298.15-892 K: $\Delta Hr° = -72.460 + 3.905\times10^{-3}T + 3.117\times10^{-6}T^2 + 6.900T^{-1}$
$\Delta Gr° = -72.460 - 3.905\times10^{-3}T\ln T - 3.117\times10^{-6}T^2 + 3.450T^{-1} + 83.720\times10^{-3}T$
892-903.9 K: $\Delta Hr° = -61.585 + 23.925\times10^{-3}T - 3.234\times10^{-6}T^2 + 6.900T^{-1}$
$\Delta Gr° = -61.585 - 23.925\times10^{-3}T\ln T + 3.234\times10^{-6}T^2 + 3.450T^{-1} + 201.869\times10^{-3}T$
903.9-1000 K: $\Delta Hr° = -68.592 + 19.101\times10^{-3}T - 0.889\times10^{-6}T^2 - 36.300T^{-1}$
$\Delta Gr° = -68.592 - 19.101\times10^{-3}T\ln T + 0.889\times10^{-6}T^2 - 18.150T^{-1} + 178.931\times10^{-3}T$

Source: Data from Mills (332) who estimated all above 298 K except temperature and enthalpy of fusion.

$ScN(c)$
Scandium Nitride
[Formation: $Sc(c,l) + 0.5N_2(g) = ScN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.863	7.100	7.100	0	-75.000	-67.825	49.716
300	8.896	7.155	7.100	.017	-75.001	-67.779	49.376
400	10.095	9.900	7.465	.974	-75.013	-65.369	35.716
500	10.720	12.226	8.190	2.018	-74.956	-62.962	27.520
600	11.119	14.218	9.033	3.111	-74.868	-60.573	22.064
700	11.411	15.955	9.901	4.238	-74.771	-58.196	18.169
800	11.646	17.495	10.756	5.391	-74.674	-55.831	15.252
900	11.848	18.878	11.582	6.566	-74.587	-53.492	12.990
1000	12.030	20.136	12.376	7.760	-74.513	-51.155	11.180
1100	12.198	21.291	13.135	8.972	-74.455	-48.816	9.699
1200	12.357	22.359	13.860	10.199	-74.418	-46.460	8.461
1300	12.510	23.354	14.552	11.443	-74.401	-44.152	7.423
1400	12.658	24.287	15.215	12.701	-74.412	-41.835	6.531
1500	12.802	25.165	15.849	13.974	-74.448	-39.501	5.755
1600	12.944	25.996	16.457	15.262	-74.511	-37.174	5.078
1608	12.955	26.061	16.505	15.366	-74.517	-36.980	5.026
1608	12.955	26.061	16.505	15.366	-75.475	-36.980	5.026
1700	13.084	26.785	17.042	16.563	-75.638	-34.783	4.472
1800	13.222	27.536	17.604	17.878	-75.804	-32.381	3.932
1812	13.238	27.624	17.670	18.037	-75.823	-32.092	3.871
1812	13.238	27.624	17.670	18.037	-79.192	-32.092	3.871
1900	13.359	28.255	18.146	19.207	-79.327	-29.803	3.428
2000	13.495	28.944	18.669	20.550	-79.471	-27.198	2.972

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1608 K, α - β transition point of Sc; ΔH° = 0.958 kcal/mol.
1812 K, melting point of Sc; ΔH° = 3.369 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.950 + 1.300\times10^{-3}T - 2.200\times10^{5}T^{-2}$
$H°-H°_{298} = 10.950\times10^{-3}T + 0.650\times10^{-6}T^2 + 2.200\times10^{2}T^{-1} - 4.060$

Formation equations (kcal/mol):

298.15-1608 K: $\Delta Hf° = -76.625 + 2.807\times10^{-3}T - 0.984\times10^{-6}T^2 + 261.050T^{-1}$
$\Delta Gf° = -76.625 - 2.807\times10^{-3}T\ln T + 0.984\times10^{-6}T^2 + 130.525T^{-1} + 43.750\times10^{-3}T$
1608-1812 K: $\Delta Hf° = -71.879 - 2.879\times10^{-3}T + 0.355\times10^{-6}T^2 + 223.950T^{-1}$
$\Delta Gf° = -71.879 + 2.879\times10^{-3}T\ln T - 0.355\times10^{-6}T^2 + 111.975T^{-1} + 0.981\times10^{-3}T$
1812-2000 K: $\Delta Hf° = -75.248 - 2.879\times10^{-3}T + 0.355\times10^{-6}T^2 + 223.950T^{-1}$
$\Delta Gf° = -75.248 + 2.879\times10^{-3}T\ln T - 0.355\times10^{-6}T^2 + 111.975T^{-1} + 2.840\times10^{-3}T$

Source: Data from Barin (23) who estimated all except enthalpy of formation at 298 K.

ScO(g)
Scandium Monoxide (ideal gas)
[Formation: Sc(c,l) + $0.5O_2(g)$ = ScO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.440	53.647	53.647	0	-13.000	-19.221	14.089
300	7.440	53.694	53.647	.014	-13.003	-19.258	14.030
400	7.760	55.872	53.942	.772	-13.221	-21.312	11.644
500	8.060	57.638	54.510	1.564	-13.430	-23.309	10.188
600	8.280	59.129	55.159	2.382	-13.639	-25.267	9.203
700	8.430	60.417	55.820	3.218	-13.858	-27.185	8.487
800	8.550	61.551	56.467	4.067	-14.093	-29.069	7.941
900	8.630	62.562	57.089	4.926	-14.349	-30.938	7.513
1000	8.700	63.476	57.683	5.793	-14.628	-32.769	7.162
1100	8.750	64.307	58.248	6.665	-14.936	-34.562	6.867
1200	8.790	65.070	58.785	7.542	-15.273	-36.304	6.612
1300	8.820	65.775	59.296	8.423	-15.641	-38.065	6.399
1400	8.850	66.431	59.783	9.307	-16.048	-39.784	6.210
1500	8.870	67.042	60.247	10.193	-16.491	-41.459	6.040
1600	8.900	67.616	60.690	11.082	-16.974	-43.112	5.889
1608	8.901	67.660	60.724	11.153	-17.014	-43.236	5.876
1608	8.901	67.660	60.724	11.153	-17.972	-43.236	5.876
1700	8.910	68.155	61.113	11.972	-18.531	-44.674	5.743
1800	8.930	68.666	61.519	12.864	-19.140	-46.203	5.610
1812	8.932	68.725	61.567	12.971	-19.213	-46.383	5.594
1812	8.932	68.725	61.567	12.971	-22.582	-46.383	5.594
1900	8.950	69.149	61.908	13.758	-23.119	-47.527	5.467
2000	8.960	69.608	62.281	14.654	-23.730	-48.800	5.332

Phase changes: 1608 K, α - β transition point of Sc; ΔH° = 0.958 kcal/mol.
1812 K, melting point of Sc; ΔH° = 3.369 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.163 + 0.522\times10^{-3}T - 0.781\times10^{5}T^{-2}$
$H°-H°_{298} = 8.163\times10^{-3}T + 0.261\times10^{-6}T^{2} + 0.781\times10^{2}T^{-1} - 2.719$

Formation equations (kcal/mol):

298.15-1608 K: $\Delta Hf° = -13.092 - 0.336\times10^{-3}T - 1.329\times10^{-6}T^{2} + 92.600T^{-1}$
$\Delta Gf° = -13.092 + 0.336\times10^{-3}T\ln T + 1.329\times10^{-6}T^{2} + 46.300T^{-1} - 23.387\times10^{-3}T$
1608-1812 K: $\Delta Hf° = -8.346 - 6.022\times10^{-3}T + 0.010\times10^{-6}T^{2} + 55.500T^{-1}$
$\Delta Gf° = -8.346 + 6.022\times10^{-3}T\ln T - 0.010\times10^{-6}T^{2} + 27.750T^{-1} - 66.156\times10^{-3}T$
1812-2000 K: $\Delta Hf° = -11.715 - 6.022\times10^{-3}T + 0.010\times10^{-6}T^{2} + 55.500T^{-1}$
$\Delta Gf° = -11.715 + 6.022\times10^{-3}T\ln T - 0.010\times10^{-6}T^{2} + 27.750T^{-1} - 64.297\times10^{-3}T$

Source: Data from Pedley (396).

$ScO_2(g)$
Scandium Dioxide (ideal gas)
[Formation: $Sc(c,l) + O_2(g) = ScO_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.150	62.732	62.732	0	-98.869	-100.493	73.662
300	10.172	62.794	62.732	.019	-98.874	-100.502	73.214
400	11.209	65.871	63.144	1.091	-99.133	-101.005	55.186
500	11.933	68.455	63.955	2.250	-99.340	-101.447	44.342
600	12.424	70.677	64.895	3.469	-99.525	-101.853	37.099
700	12.762	72.619	65.862	4.730	-99.708	-102.223	31.915
800	13.001	74.339	66.815	6.019	-99.902	-102.565	28.019
900	13.175	75.881	67.739	7.328	-100.115	-102.898	24.987
1000	13.304	77.277	68.625	8.652	-100.351	-103.198	22.554
1100	13.403	78.549	69.469	9.988	-100.614	-103.462	20.556
1200	13.480	79.719	70.276	11.332	-100.908	-103.681	18.883
1300	13.541	80.801	71.045	12.683	-101.235	-103.923	17.471
1400	13.590	81.806	71.777	14.040	-101.600	-104.124	16.254
1500	13.630	82.745	72.478	15.401	-102.003	-104.286	15.194
1600	13.663	83.626	73.147	16.766	-102.449	-104.428	14.264
1608	13.665	83.694	73.200	16.875	-102.486	-104.430	14.193
1608	13.665	83.694	73.200	16.875	-103.444	-104.430	14.193
1700	13.690	84.455	73.789	18.133	-103.970	-104.482	13.432
1800	13.713	85.238	74.402	19.504	-104.544	-104.501	12.688
1812	13.715	85.329	74.475	19.669	-104.613	-104.501	12.604
1812	13.715	85.329	74.475	19.669	-107.982	-104.501	12.604
1900	13.733	85.980	74.993	20.876	-108.492	-104.322	12.000
2000	13.750	86.685	75.560	22.250	-109.074	-104.092	11.374

Phase changes: 1608 K, α - β transition point of Sc; ΔH° = 0.958 kcal/mol.
1812 K, melting point of Sc; ΔH° = 3.369 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.563 + 0.824\times10^{-3}T - 2.364\times10^{5}T^{-2}$
$H°-H°_{298} = 12.563\times10^{-3}T + 0.412\times10^{-6}T^{2} + 2.364\times10^{2}T^{-1} - 4.575$

Formation equations (kcal/mol):

298.15-1608 K: $\Delta Hf° = -99.641 + 0.449\times10^{-3}T - 1.430\times10^{-6}T^{2} + 228.300T^{-1}$
$\Delta Gf° = -99.641 - 0.449\times10^{-3}T\ln T + 1.430\times10^{-6}T^{2} + 114.150T^{-1} - 2.008\times10^{-3}T$
1608-1812 K: $\Delta Hf° = -94.896 - 5.237\times10^{-3}T - 0.091\times10^{-6}T^{2} + 191.200T^{-1}$
$\Delta Gf° = -94.896 + 5.237\times10^{-3}T\ln T + 0.091\times10^{-6}T^{2} + 95.600T^{-1} - 44.778\times10^{-3}T$
1812-2000 K: $\Delta Hf° = -98.265 - 5.237\times10^{-3}T - 0.091\times10^{-6}T^{2} + 191.200T^{-1}$
$\Delta Gf° = -98.265 + 5.237\times10^{-3}T\ln T + 0.091\times10^{-6}T^{2} + 95.600T^{-1} - 42.919\times10^{-3}T$

Source: Data from Gurvich (193).

$Sc_2O(g)$
Discandium Oxide (ideal gas)
[Formation: $2Sc(c,l) + 0.5O_2(g) = Sc_2O(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.120	64.597	64.597	0	-5.508	-12.525	9.181
300	11.138	64.666	64.597	.021	-5.516	-12.566	9.154
400	11.919	67.984	65.044	1.176	-5.957	-14.853	8.115
500	12.451	70.705	65.913	2.396	-6.373	-17.025	7.442
600	12.811	73.009	66.909	3.660	-6.785	-19.121	6.965
700	13.060	75.004	67.925	4.955	-7.211	-21.138	6.599
800	13.236	76.760	68.923	6.270	-7.665	-23.089	6.307
900	13.364	78.326	69.882	7.600	-8.158	-25.011	6.074
1000	13.460	79.740	70.798	8.942	-8.695	-26.860	5.870
1100	13.533	81.026	71.670	10.292	-9.285	-28.635	5.689
1200	13.590	82.206	72.499	11.648	-9.933	-30.311	5.520
1300	13.635	83.296	73.289	13.009	-10.644	-32.028	5.384
1400	13.672	84.308	74.040	14.375	-11.426	-33.660	5.254
1500	13.701	85.252	74.757	15.743	-12.280	-35.209	5.130
1600	13.726	86.137	75.440	17.115	-13.215	-36.715	5.015
1608	13.728	86.205	75.494	17.225	-13.292	-36.817	5.004
1608	13.728	86.205	75.494	17.225	-15.208	-36.817	5.004
1700	13.746	86.970	76.095	18.488	-16.295	-38.043	4.891
1800	13.764	87.756	76.720	19.864	-17.477	-39.302	4.772
1812	13.766	87.847	76.794	20.029	-17.619	-39.447	4.758
1812	13.766	87.847	76.794	20.029	-24.357	-39.447	4.758
1900	13.778	88.501	77.322	21.241	-25.399	-40.159	4.619
2000	13.791	89.208	77.898	22.619	-26.584	-40.915	4.471

Phase changes: 1608 K, α - β transition point of Sc; ΔH° = 0.958 kcal/mol.
1812 K, melting point of Sc; ΔH° = 3.369 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.926 + 0.600\times10^{-3}T - 1.764\times10^{5}T^{-2}$
$H°-H°_{298} = 12.926\times10^{-3}T + 0.300\times10^{-6}T^{2} + 1.764\times10^{2}T^{-1} - 4.472$

Formation equations (kcal/mol):

298.15-1608 K: $\Delta Hf° = -5.903 - 0.457\times10^{-3}T - 2.629\times10^{-6}T^{2} + 228.000T^{-1}$
$\Delta Gf° = -5.903 + 0.457\times10^{-3}T\ln T + 2.629\times10^{-6}T^{2} + 114.000T^{-1} - 26.881\times10^{-3}T$
1608-1812 K: $\Delta Hf° = 3.589 - 11.829\times10^{-3}T + 0.049\times10^{-6}T^{2} + 153.800T^{-1}$
$\Delta Gf° = 3.589 + 11.829\times10^{-3}T\ln T - 0.049\times10^{-6}T^{2} + 76.900T^{-1} - 112.420\times10^{-3}T$
1812-2000 K: $\Delta Hf° = -3.149 - 11.829\times10^{-3}T + 0.049\times10^{-6}T^{2} + 153.800T^{-1}$
$\Delta Gf° = -3.149 + 11.829\times10^{-3}T\ln T - 0.049\times10^{-6}T^{2} + 76.900T^{-1} - 108.701\times10^{-3}T$

Source: Data from Gurvich (193).

$Sc_2O_2(g)$
Discandium Dioxide (ideal gas)
[Formation: $2Sc(c,l) + O_2(g) = Sc_2O_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.406	67.657	67.657	0	-117.253	-117.877	86.405
300	13.440	67.740	67.657	.025	-117.263	-117.878	85.873
400	15.065	71.840	68.205	1.454	-117.786	-118.006	64.475
500	16.262	75.337	69.291	3.023	-118.218	-118.006	51.580
600	17.111	78.382	70.559	4.694	-118.600	-117.931	42.956
700	17.714	81.068	71.872	6.437	-118.967	-117.785	36.774
800	18.149	83.463	73.173	8.232	-119.340	-117.582	32.122
900	18.470	85.620	74.439	10.063	-119.739	-117.364	28.499
1000	18.712	87.579	75.656	11.923	-120.172	-117.081	25.588
1100	18.897	89.371	76.822	13.804	-120.650	-116.735	23.193
1200	19.043	91.022	77.938	15.701	-121.181	-116.302	21.181
1300	19.158	92.551	79.004	17.611	-121.771	-115.918	19.487
1400	19.252	93.975	80.024	19.532	-122.430	-115.461	18.024
1500	19.328	95.305	80.998	21.461	-123.159	-114.927	16.745
1600	19.392	96.555	81.932	23.397	-123.968	-114.362	15.621
1608	19.396	96.652	82.005	23.552	-124.035	-114.298	15.534
1608	19.396	96.652	82.005	23.552	-125.951	-114.298	15.534
1700	19.445	97.732	82.827	25.339	-126.920	-113.623	14.607
1800	19.489	98.845	83.686	27.286	-127.975	-112.824	13.699
1812	19.494	98.975	83.787	27.520	-128.102	-112.722	13.596
1812	19.494	98.975	83.787	27.520	-134.840	-112.722	13.596
1900	19.527	99.900	84.512	29.237	-135.770	-111.631	12.840
2000	19.560	100.902	85.307	31.191	-136.829	-110.341	12.057

Phase changes: 1608 K, α - β transition point of Sc; ΔH° = 0.958 kcal/mol.
1812 K, melting point of Sc; ΔH° = 3.369 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 17.112 + 1.670\times10^{-3}T - 3.737\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.112\times10^{-3}T + 0.835\times10^{-6}T^{2} + 3.737\times10^{2}T^{-1} - 6.430$

Formation equations (kcal/mol):

298.15-1608 K: $\Delta Hf^\circ = -118.429 + 0.114\times10^{-3}T - 2.346\times10^{-6}T^{2} + 402.700T^{-1}$
$\Delta Gf^\circ = -118.429 - 0.114\times10^{-3}T\ln T + 2.346\times10^{-6}T^{2} + 201.350T^{-1} - 0.462\times10^{-3}T$
1608-1812 K: $\Delta Hf^\circ = -108.937 - 11.258\times10^{-3}T + 0.332\times10^{-6}T^{2} + 328.500T^{-1}$
$\Delta Gf^\circ = -108.937 + 11.258\times10^{-3}T\ln T - 0.332\times10^{-6}T^{2} + 164.250T^{-1} - 86.001\times10^{-3}T$
1812-2000 K: $\Delta Hf^\circ = -115.675 - 11.258\times10^{-3}T + 0.332\times10^{-6}T^{2} + 328.500T^{-1}$
$\Delta Gf^\circ = -115.675 + 11.258\times10^{-3}T\ln T - 0.332\times10^{-6}T^{2} + 164.250T^{-1} - 82.283\times10^{-3}T$

Source: Data from Gurvich (193).

$ScPO_4(c)$
Scandium Phosphate
[Formation: $Sc(c,l) + P(c,l,1/4P_4(g)) + 2O_2(g) = ScPO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	22.242	20.000	20.000	0	-454.000	-425.345	311.782
300	22.394	20.138	20.001	.041	-454.007	-425.167	309.730
317.3	23.327	21.420	20.044	.436	-454.060	-423.501	291.695
317.3	23.327	21.420	20.044	.436	-454.217	-423.501	291.695
400	27.786	27.426	20.956	2.588	-454.277	-415.483	227.006
500	30.375	33.935	22.917	5.509	-454.082	-405.801	177.373
550	31.118	36.875	24.052	7.053	-453.925	-400.996	159.339
550	31.118	36.875	24.052	7.053	-456.833	-400.996	159.339
600	31.860	39.615	25.237	8.627	-456.579	-395.930	144.215
700	32.823	44.603	27.654	11.864	-456.036	-385.861	120.470
800	33.509	49.033	30.056	15.182	-455.477	-375.872	102.682
900	34.033	53.012	32.390	18.560	-454.917	-365.967	88.868
1000	34.457	56.620	34.634	21.986	-454.363	-356.115	77.828
1100	34.816	59.921	36.785	25.450	-453.824	-346.309	68.804
1200	35.130	62.964	38.842	28.947	-453.302	-336.531	61.290
1300	35.412	65.788	40.807	32.475	-452.798	-326.845	54.947
1400	35.672	68.422	42.687	36.029	-452.321	-317.183	49.514
1500	35.914	70.891	44.486	39.608	-451.868	-307.543	44.808
1600	36.144	73.216	46.209	43.211	-451.445	-297.938	40.696
1608*	36.162	73.396	46.344	43.500	-451.412	-297.162	40.388
1608	36.162	73.396	46.344	43.500	-452.370	-297.162	40.388
1700	36.364	75.414	47.863	46.837	-452.082	-288.299	37.063
1800	36.577	77.499	49.452	50.484	-451.761	-278.680	33.836

*Data extrapolated above 1600 K

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.
1608 K, α - β transition point of Sc; ΔH° = 0.958 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp^\circ = 33.807 + 1.724\times10^{-3}T - 10.738\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 33.807\times10^{-3}T + 0.862\times10^{-6}T^2 + 10.738\times10^{2}T^{-1} - 13.758$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf^\circ = -460.187 + 10.664\times10^{-3}T - 4.668\times10^{-6}T^2 + 1020.500T^{-1}$
$\Delta Gf^\circ = -460.187 - 10.664\times10^{-3}T\ln T + 4.668\times10^{-6}T^2 + 510.250T^{-1} + 170.490\times10^{-3}T$
317.3-550 K: $\Delta Hf^\circ = -459.874 + 8.171\times10^{-3}T - 1.483\times10^{-6}T^2 + 1020.500T^{-1}$
$\Delta Gf^\circ = -459.874 - 8.171\times10^{-3}T\ln T + 1.483\times10^{-6}T^2 + 510.250T^{-1} + 156.153\times10^{-3}T$
550-1608 K: $\Delta Hf^\circ = -463.334 + 9.509\times10^{-3}T - 1.487\times10^{-6}T^2 + 920.200T^{-1}$
$\Delta Gf^\circ = -463.334 - 9.509\times10^{-3}T\ln T + 1.487\times10^{-6}T^2 + 460.100T^{-1} + 171.051\times10^{-3}T$
1608-1800 K: $\Delta Hf^\circ = -458.588 + 3.823\times10^{-3}T - 0.148\times10^{-6}T^2 + 883.100T^{-1}$
$\Delta Gf^\circ = -458.588 - 3.823\times10^{-3}T\ln T + 0.148\times10^{-6}T^2 + 441.550T^{-1} + 128.281\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Rat'kovskii (417). Other data based on Tsagareishvili (503).

SiC(hexagonal)
α-Silicon Carbide

[Formation: Si(c,l) + C(c) = SiC(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	6.380	3.940	3.940	0	-15.000	-14.424	10.573
300	6.425	3.980	3.940	.012	-15.001	-14.420	10.505
400	8.258	6.117	4.220	.759	-15.005	-14.227	7.773
500	9.321	8.082	4.798	1.642	-14.985	-14.032	6.134
600	10.063	9.851	5.496	2.613	-14.963	-13.845	5.043
700	10.619	11.446	6.235	3.648	-14.943	-13.662	4.265
800	11.046	12.893	6.978	4.732	-14.923	-13.478	3.682
900	11.379	14.214	7.710	5.854	-14.908	-13.300	3.230
1000	11.638	15.427	8.421	7.006	-14.891	-13.113	2.866
1100	11.838	16.546	9.110	8.180	-14.878	-12.933	2.570
1200	11.990	17.583	9.773	9.372	-14.868	-12.768	2.325
1300	12.103	18.547	10.411	10.577	-14.863	-12.593	2.117
1400	12.186	19.447	11.025	11.791	-14.865	-12.415	1.938
1500	12.246	20.290	11.615	13.013	-14.874	-12.251	1.785
1600	12.288	21.082	12.182	14.240	-14.889	-12.076	1.650
1687	12.315	21.733	12.658	15.310	-14.911	-11.904	1.542
1687	12.315	21.733	12.658	15.310	-26.993	-11.904	1.542
1700	12.319	21.828	12.728	15.470	-26.988	-11.783	1.515
1800	12.342	22.533	13.254	16.703	-26.952	-10.887	1.322
1900	12.362	23.201	13.759	17.939	-26.918	-9.995	1.150
2000	12.383	23.835	14.247	19.176	-26.889	-9.109	.995

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2900 K: $Cp^\circ = 11.127 + 0.710\times10^{-3}T - 4.408\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 11.127\times10^{-3}T + 0.355\times10^{-6}T^{2} + 4.408\times10^{2}T^{-1} - 4.828$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf^\circ = -16.078 + 1.930\times10^{-3}T - 0.762\times10^{-6}T^{2} + 170.000T^{-1}$

$\Delta Gf^\circ = -16.078 - 1.930\times10^{-3}T\ln T + 0.762\times10^{-6}T^{2} + 85.000T^{-1} + 15.360\times10^{-3}T$

1687-2000 K: $\Delta Hf^\circ = -28.507 + 1.509\times10^{-3}T - 0.411\times10^{-6}T^{2} + 268.500T^{-1}$

$\Delta Gf^\circ = -28.507 - 1.509\times10^{-3}T\ln T + 0.411\times10^{-6}T^{2} + 134.250T^{-1} + 20.174\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K based on Humphrey (211). High-temperature data based on Humphrey (211) and Chekhovsky (85).

SiC(cubic)
β-Silicon Carbide
[Formation: $Si(c,l) + C(c) = SiC(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$C_p°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	6.420	3.960	3.960	0	-15.600	-15.030	11.017
300	6.469	4.000	3.960	.012	-15.601	-15.026	10.947
400	8.322	6.145	4.240	.762	-15.602	-14.835	8.105
500	9.362	8.123	4.823	1.650	-15.577	-14.645	6.401
600	10.055	9.895	5.523	2.623	-15.553	-14.462	5.268
700	10.565	11.485	6.264	3.655	-15.536	-14.282	4.459
800	10.960	12.922	7.007	4.732	-15.523	-14.101	3.852
900	11.275	14.232	7.738	5.845	-15.517	-13.925	3.381
1000	11.529	15.434	8.449	6.985	-15.512	-13.741	3.003
1100	11.736	16.543	9.135	8.149	-15.509	-13.561	2.694
1200	11.903	17.571	9.795	9.331	-15.509	-13.395	2.439
1300	12.037	18.529	10.431	10.528	-15.512	-13.219	2.222
1400	12.143	19.425	11.041	11.737	-15.519	-13.038	2.035
1500	12.225	20.266	11.629	12.956	-15.531	-12.872	1.875
1600	12.288	21.057	12.193	14.182	-15.547	-12.694	1.734
1687	12.330	21.709	12.668	15.253	-15.568	-12.521	1.622
1687	12.330	21.709	12.668	15.253	-27.650	-12.521	1.622
1700	12.336	21.804	12.738	15.413	-27.645	-12.399	1.594
1800	12.371	22.510	13.261	16.649	-27.606	-11.500	1.396
1900	12.396	23.179	13.765	17.887	-27.570	-10.605	1.220
2000	12.416	23.816	14.252	19.128	-27.537	-9.719	1.062

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p° = 10.504 + 1.238\times10^{-3}T - 3.958\times10^{5}T^{-2}$

$H°-H°_{298} = 10.504\times10^{-3}T + 0.619\times10^{-6}T^{2} + 3.958\times10^{2}T^{-1} - 4.514$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -16.365 + 1.307\times10^{-3}T - 0.498\times10^{-6}T^{2} + 125.000T^{-1}$

$\Delta Gf° = -16.365 - 1.307\times10^{-3}T\ln T + 0.498\times10^{-6}T^{2} + 62.500T^{-1} + 11.072\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -28.794 + 0.886\times10^{-3}T - 0.147\times10^{-6}T^{2} + 223.500T^{-1}$

$\Delta Gf° = -28.794 - 0.886\times10^{-3}T\ln T + 0.147\times10^{-6}T^{2} + 111.750T^{-1} + 15.886\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K on Humphrey (211) and Koshchenko (281). High-temperature data based based on Humphrey (211).

$SiC(g)$
Silicon Monocarbide (ideal gas)
[Formation: $Si(c,l) + C(c) = SiC(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	9.182	50.892	50.892	0	172.000	158.577	-116.239
300	9.216	50.949	50.892	.017	172.004	158.494	-115.461
400	10.574	53.813	51.273	1.016	172.252	153.952	-84.114
500	10.857	56.219	52.029	2.095	172.468	149.352	-65.281
600	10.610	58.180	52.897	3.170	172.594	144.714	-52.712
700	10.264	59.790	53.770	4.214	172.623	140.063	-43.729
800	9.972	61.140	54.609	5.225	172.570	135.417	-36.994
900	9.761	62.302	55.401	6.211	172.449	130.778	-31.757
1000	9.620	63.323	56.144	7.179	172.282	126.164	-27.573
1100	9.532	64.235	56.838	8.137	172.079	121.566	-24.153
1200	9.483	65.062	57.489	9.087	171.847	116.972	-21.303
1300	9.460	65.820	58.102	10.034	171.594	112.409	-18.897
1400	9.455	66.521	58.678	10.980	171.324	107.870	-16.839
1500	9.462	67.173	59.223	11.925	171.038	103.337	-15.056
1600	9.477	67.784	59.739	12.872	170.743	98.833	-13.500
1687	9.494	68.287	60.168	13.698	170.476	94.948	-12.300
1687	9.494	68.287	60.168	13.698	158.394	94.948	-12.300
1700	9.497	68.360	60.230	13.821	158.363	94.463	-12.144
1800	9.520	68.903	60.696	14.772	158.117	90.716	-11.014
1900	9.544	69.418	61.142	15.725	157.868	86.979	-10.005
2000	9.567	69.909	61.568	16.681	157.616	83.248	-9.097

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.631 - 1.326\text{x}10^{-3}T - 1.822\text{x}10^{5}T^{-2}$

$H°-H°_{298} = 11.631\text{x}10^{-3}T - 0.663\text{x}10^{-6}T^{2} + 1.822\text{x}10^{2}T^{-1} - 4.020$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = 171.730 + 2.434\text{x}10^{-3}T - 1.780\text{x}10^{-6}T^{2} - 88.600T^{-1}$

$\Delta Gf° = 171.730 - 2.434\text{x}10^{-3}T\ln T + 1.780\text{x}10^{-6}T^{2} - 44.300T^{-1} - 30.278\text{x}10^{-3}T$

1687-2000 K: $\Delta Hf° = 159.301 + 2.013\text{x}10^{-3}T - 1.429\text{x}10^{-6}T^{2} + 9.900T^{-1}$

$\Delta Gf° = 159.301 - 2.013\text{x}10^{-3}T\ln T + 1.429\text{x}10^{-6}T^{2} + 4.950T^{-1} - 25.464\text{x}10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$SiC_2(g)$
Silicon Dicarbide (ideal gas)
[Formation: $Si(c,l) + 2C(c) = SiC_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	10.901	56.553	56.553	0	147.000	132.299	-96.976
300	10.917	56.620	56.553	.020	147.003	132.207	-96.312
400	11.671	59.869	56.992	1.151	147.139	127.250	-69.525
500	12.259	62.539	57.841	2.349	147.157	122.274	-53.445
600	12.729	64.817	58.819	3.599	147.081	117.304	-42.727
700	13.105	66.809	59.820	4.892	146.935	112.350	-35.077
800	13.403	68.579	60.807	6.218	146.738	107.425	-29.347
900	13.641	70.172	61.761	7.570	146.496	102.522	-24.895
1000	13.831	71.619	62.675	8.944	146.228	97.659	-21.343
1100	13.984	72.945	63.550	10.335	145.934	92.829	-18.443
1200	14.109	74.167	64.384	11.740	145.619	87.994	-16.026
1300	14.212	75.301	65.181	13.156	145.285	83.203	-13.988
1400	14.298	76.357	65.941	14.582	144.936	78.446	-12.246
1500	14.372	77.346	66.669	16.015	144.570	73.698	-10.738
1600	14.438	78.276	67.366	17.456	144.195	68.985	-9.423
1687	14.490	79.042	67.948	18.715	143.855	64.924	-8.411
1687	14.490	79.042	67.948	18.715	131.773	64.924	-8.411
1700	14.498	79.153	68.034	18.903	131.731	64.413	-8.281
1800	14.557	79.983	68.674	20.356	131.400	60.467	-7.342
1900	14.616	80.772	69.291	21.814	131.064	56.535	-6.503
2000	14.677	81.523	69.884	23.279	130.723	52.617	-5.750

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 12.571 + 1.196\times10^{-3}T - 1.802\times10^{5}T^{-2}$
$H°- H°_{298} = 12.571\times10^{-3}T + 0.598\times10^{-6}T^{2} + 1.802\times10^{2}T^{-1} - 4.406$

Formation equations (kcal/mol):

298.15-1687 K: $ΔHf° = 148.039 - 0.144\times10^{-3}T - 1.285\times10^{-6}T^{2} - 262.900T^{-1}$
$ΔGf° = 148.039 + 0.144\times10^{-3}T\ln T + 1.285\times10^{-6}T^{2} - 131.450T^{-1} - 52.518\times10^{-3}T$
1687-2000 K: $ΔHf° = 135.610 - 0.565\times10^{-3}T - 0.934\times10^{-6}T^{2} - 164.400T^{-1}$
$ΔGf° = 135.610 + 0.565\times10^{-3}T\ln T + 0.934\times10^{-6}T^{2} - 82.200T^{-1} - 47.704\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$Si_2C(g)$
Disilicon Carbide (ideal gas)
[Formation: $2Si(c,l) + C(c) = Si_2C(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.334	57.881	57.881	0	128.000	113.835	-83.442
300	11.351	57.951	57.881	.021	127.999	113.747	-82.864
400	12.082	61.322	58.334	1.195	127.915	109.003	-59.556
500	12.630	64.080	59.218	2.431	127.742	104.295	-45.587
600	13.057	66.422	60.227	3.717	127.507	99.626	-36.288
700	13.391	68.461	61.261	5.040	127.224	94.999	-29.660
800	13.652	70.267	62.277	6.392	126.907	90.421	-24.701
900	13.857	71.887	63.256	7.768	126.556	85.880	-20.854
1000	14.019	73.356	64.194	9.162	126.187	81.396	-17.789
1100	14.149	74.698	65.088	10.571	125.798	76.932	-15.285
1200	14.254	75.934	65.941	11.991	125.392	72.495	-13.203
1300	14.341	77.078	66.754	13.421	124.972	68.104	-11.449
1400	14.416	78.144	67.530	14.859	124.537	63.753	-9.952
1500	14.482	79.141	68.272	16.304	124.088	59.405	-8.655
1600	14.543	80.077	68.980	17.755	123.629	55.106	-7.527
1687	14.596	80.849	69.573	19.023	123.219	51.431	-6.663
1687	14.596	80.849	69.573	19.023	99.055	51.431	-6.663
1700	14.604	80.961	69.659	19.213	99.011	51.073	-6.566
1800	14.666	81.797	70.310	20.676	98.667	48.269	-5.861
1900	14.733	82.592	70.936	22.146	98.325	45.478	-5.231
2000	14.806	83.349	71.537	23.623	97.984	42.696	-4.666

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K:

$$Cp° = 13.064 + 0.950\times10^{-3}T - 1.790\times10^{5}T^{-2}$$

$$H°- H°_{298} = 13.064\times10^{-3}T + 0.475\times10^{-6}T^{2} + 1.790\times10^{2}T^{-1} - 4.538$$

Formation equations (kcal/mol):

298.15-1687 K:

$$\Delta Hf° = 129.267 - 1.812\times10^{-3}T - 0.993\times10^{-6}T^{2} - 190.300T^{-1}$$

$$\Delta Gf° = 129.267 + 1.812\times10^{-3}T\ln T + 0.993\times10^{-6}T^{2} - 95.150T^{-1} - 61.308\times10^{-3}T$$

1687-2000 K:

$$\Delta Hf° = 104.409 - 2.654\times10^{-3}T - 0.291\times10^{-6}T^{2} + 6.700T^{-1}$$

$$\Delta Gf° = 104.409 + 2.654\times10^{-3}T\ln T + 0.291\times10^{-6}T^{2} + 3.350T^{-1} - 51.679\times10^{-3}T$$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

SiH(g)
Silicon Monohydride (ideal gas)
[Formation: Si(c,l) + $0.5H_2(g)$ = SiH(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.191	47.306	47.306	0	90.000	81.890	-60.026
300	7.190	47.350	47.307	.013	89.997	81.839	-59.619
400	7.180	49.414	47.587	.731	89.862	79.137	-43.238
500	7.285	51.026	48.120	1.453	89.688	76.477	-33.427
600	7.451	52.368	48.718	2.190	89.503	73.851	-26.900
700	7.636	53.531	49.325	2.944	89.315	71.256	-22.247
800	7.817	54.562	49.916	3.717	89.130	68.691	-18.765
900	7.983	55.493	50.485	4.507	88.945	66.147	-16.062
1000	8.129	56.342	51.029	5.313	88.764	63.632	-13.906
1100	8.257	57.122	51.547	6.132	88.583	61.120	-12.143
1200	8.369	57.846	52.043	6.964	88.402	58.631	-10.678
1300	8.465	58.520	52.516	7.805	88.220	56.156	-9.441
1400	8.550	59.150	52.967	8.656	88.036	53.701	-8.383
1500	8.624	59.743	53.400	9.515	87.849	51.244	-7.466
1600	8.690	60.301	53.813	10.381	87.658	48.809	-6.667
1687	8.740	60.763	54.160	11.139	87.489	46.723	-6.053
1687	8.740	60.763	54.160	11.139	75.407	46.723	-6.053
1700	8.748	60.830	54.211	11.253	75.390	46.505	-5.979
1800	8.801	61.331	54.592	12.130	75.258	44.812	-5.441
1900	8.848	61.809	54.960	13.013	75.129	43.124	-4.960
2000	8.891	62.264	55.314	13.900	74.998	41.437	-4.528

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 6.690 + 1.304\times10^{-3}T + 0.100\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 6.690\times10^{-3}T + 0.652\times10^{-6}T^{2} - 0.100\times10^{2}T^{-1} - 2.019$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf^\circ = 90.989 - 2.217\times10^{-3}T + 0.092\times10^{-6}T^{2} - 100.250T^{-1}$
$\Delta Gf^\circ = 90.989 + 2.217\times10^{-3}T\ln T - 0.092\times10^{-6}T^{2} - 50.125T^{-1} - 42.560\times10^{-3}T$
1687-2000 K: $\Delta Hf^\circ = 78.560 - 2.638\times10^{-3}T + 0.443\times10^{-6}T^{2} - 1.750T^{-1}$
$\Delta Gf^\circ = 78.560 + 2.638\times10^{-3}T\ln T - 0.443\times10^{-6}T^{2} - 0.875T^{-1} - 37.746\times10^{-3}T$

Source: Data from Chase (80).

$SiH_2(g)$
Silicon Dihydride (ideal gas)
[Formation: $Si(c,l) + H_2(g) = SiH_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.485	49.579	49.579	0	58.640	54.504	-39.952
300	8.498	49.631	49.579	.016	58.634	54.479	-39.687
400	9.413	52.193	49.923	.908	58.325	53.139	-29.033
500	10.535	54.413	50.603	1.905	58.077	51.874	-22.674
600	11.576	56.428	51.408	3.012	57.912	50.648	-18.448
700	12.389	58.277	52.258	4.213	57.820	49.446	-15.438
800	12.956	59.971	53.118	5.482	57.778	48.255	-13.182
900	13.325	61.520	53.968	6.797	57.762	47.065	-11.429
1000	13.554	62.937	54.795	8.142	57.761	45.884	-10.028
1100	13.691	64.235	55.594	9.505	57.761	44.690	-8.879
1200	13.771	65.430	56.365	10.878	57.754	43.502	-7.923
1300	13.817	66.535	57.106	12.258	57.738	42.314	-7.113
1400	13.842	67.560	57.816	13.641	57.708	41.132	-6.421
1500	13.855	68.515	58.498	15.026	57.663	39.939	-5.819
1600	13.862	69.410	59.153	16.412	57.604	38.756	-5.294
1687	13.865	70.144	59.700	17.618	57.540	37.756	-4.891
1687	13.865	70.144	59.700	17.618	45.458	37.756	-4.891
1700	13.865	70.250	59.781	17.798	45.456	37.701	-4.847
1800	13.866	71.043	60.385	19.185	45.436	37.246	-4.522
1900	13.866	71.793	60.966	20.572	45.407	36.792	-4.232
2000	13.866	72.504	61.525	21.958	45.368	36.334	-3.970

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.631 + 1.620 \times 10^{-3}T - 3.226 \times 10^{5}T^{-2}$

$H°-H°_{298} = 11.631 \times 10^{-3}T + 0.810 \times 10^{-6}T^{2} + 3.226 \times 10^{2}T^{-1} - 4.622$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = 57.980 - 0.504 \times 10^{-3}T + 0.040 \times 10^{-6}T^{2} + 240.600T^{-1}$

$\Delta Gf° = 57.980 + 0.504 \times 10^{-3}T\ln T - 0.040 \times 10^{-6}T^{2} + 120.300T^{-1} - 15.870 \times 10^{-3}T$

1687-2000 K: $\Delta Hf° = 45.551 - 0.925 \times 10^{-3}T + 0.391 \times 10^{-6}T^{2} + 339.100T^{-1}$

$\Delta Gf° = 45.551 + 0.925 \times 10^{-3}T\ln T - 0.391 \times 10^{-6}T^{2} + 169.550T^{-1} - 11.056 \times 10^{-3}T$

Source: Data from Gurvich (195).

$SiH_3(g)$
Silicon Trihydride (ideal gas)
[Formation: $Si(c,l) + 1.5H_2(g) = SiH_3(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.302	51.718	51.718	0	50.038	49.917	-36.589
300	9.326	51.775	51.718	.017	50.026	49.915	-36.363
400	10.640	54.637	52.100	1.015	49.476	49.962	-27.298
500	11.914	57.150	52.862	2.144	49.011	50.140	-21.916
600	13.068	59.426	53.769	3.394	48.639	50.401	-18.358
700	14.070	61.518	54.729	4.752	48.353	50.718	-15.835
800	14.919	63.454	55.700	6.203	48.140	51.073	-13.952
900	15.626	65.253	56.663	7.731	47.981	51.449	-12.493
1000	16.213	66.931	57.607	9.324	47.869	51.849	-11.331
1100	16.699	68.500	58.526	10.971	47.791	52.243	-10.380
1200	17.103	69.971	59.420	12.661	47.732	52.651	-9.589
1300	17.440	71.354	60.286	14.389	47.692	53.062	-8.920
1400	17.723	72.657	61.123	16.148	47.659	53.481	-8.349
1500	17.961	73.888	61.933	17.932	47.630	53.886	-7.851
1600	18.164	75.054	62.717	19.739	47.604	54.301	-7.417
1687	18.315	76.019	63.378	21.326	47.578	54.690	-7.085
1687	18.315	76.019	63.378	21.326	35.496	54.690	-7.085
1700	18.338	76.160	63.475	21.564	35.501	54.842	-7.050
1800	18.487	77.213	64.210	23.405	35.536	55.978	-6.797
1900	18.616	78.216	64.921	25.261	35.573	57.115	-6.570
2000	18.729	79.173	65.609	27.128	35.608	58.243	-6.364

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.277 + 4.636\text{x}10^{-3}T - 2.984\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 11.277\text{x}10^{-3}T + 2.318\text{x}10^{-6}T^{2} + 2.984\text{x}10^{2}T^{-1} - 4.569$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = 50.384 - 4.086\text{x}10^{-3}T + 1.339\text{x}10^{-6}T^{2} + 224.650T^{-1}$

$\Delta Gf° = 50.384 + 4.086\text{x}10^{-3}T\ln T - 1.339\text{x}10^{-6}T^{2} + 112.325T^{-1} - 25.712\text{x}10^{-3}T$

1687-2000 K: $\Delta Hf° = 37.955 - 4.507\text{x}10^{-3}T + 1.690\text{x}10^{-6}T^{2} + 323.150T^{-1}$

$\Delta Gf° = 37.955 + 4.507\text{x}10^{-3}T\ln T - 1.690\text{x}10^{-6}T^{2} + 161.575T^{-1} - 20.898\text{x}10^{-3}T$

Source: Data from Gurvich (195).

$SiH_4(g)$
Silicon Tetrahydride (ideal gas), Silane
[Formation: $Si(c,l) + 2H_2(g) = SiH_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.236	48.887	48.887	0	8.200	13.575	-9.950
300	10.274	48.950	48.887	.019	8.184	13.608	-9.913
400	12.302	52.186	49.313	1.149	7.419	15.534	-8.487
500	14.136	55.132	50.186	2.473	6.799	17.639	-7.710
600	15.745	57.855	51.242	3.968	6.322	19.851	-7.231
700	17.140	60.390	52.370	5.614	5.973	22.135	-6.911
800	18.335	62.759	53.521	7.390	5.732	24.464	-6.683
900	19.347	64.978	54.672	9.275	5.575	26.815	-6.511
1000	20.199	67.062	55.808	11.254	5.490	29.188	-6.379
1100	20.914	69.022	56.922	13.310	5.457	31.551	-6.269
1200	21.516	70.868	58.007	15.433	5.464	33.926	-6.179
1300	22.023	72.611	59.065	17.610	5.499	36.295	-6.102
1400	22.452	74.259	60.091	19.835	5.555	38.666	-6.036
1500	22.818	75.821	61.088	22.099	5.622	41.018	-5.976
1600	23.130	77.304	62.056	24.397	5.698	43.372	-5.924
1687	23.364	78.535	62.874	26.419	5.766	45.443	-5.887
1687	23.364	78.535	62.874	26.419	-6.316	45.443	-5.887
1700	23.399	78.714	62.995	26.723	-6.297	45.845	-5.894
1800	23.631	80.059	63.906	29.075	-6.149	48.908	-5.938
1900	23.822	81.342	64.790	31.449	-5.997	51.964	-5.977
2000	24.009	82.569	65.648	33.841	-5.845	55.005	-6.011

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.383 + 6.408\times10^{-3}T - 4.496\times10^{5}T^{-2}$
$H°-H°_{298} = 13.383\times10^{-3}T + 3.204\times10^{-6}T^{2} + 4.496\times10^{2}T^{-1} - 5.783$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = 8.285 - 5.208\times10^{-3}T + 2.015\times10^{-6}T^{2} + 384.100T^{-1}$
$\Delta Gf° = 8.285 + 5.208\times10^{-3}T\ln T - 2.015\times10^{-6}T^{2} + 192.050T^{-1} - 13.492\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -4.144 - 5.629\times10^{-3}T + 2.366\times10^{-6}T^{2} + 482.600T^{-1}$
$\Delta Gf° = -4.144 + 5.629\times10^{-3}T\ln T - 2.366\times10^{-6}T^{2} + 241.300T^{-1} - 8.678\times10^{-3}T$

Source: Data from Chase (82).

$SiHBr_3(g)$
Tribromosilane (ideal gas)
[Formation: $Si(c,l) + 0.5H_2(g) + 1.5Br_2(l,g) = SiHBr_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.218	83.158	83.158	0	-72.400	-74.930	54.925
300	19.255	83.277	83.158	.036	-72.429	-74.945	54.596
332.6	19.769	85.290	83.269	.672	-72.946	-75.192	49.407
332.6	19.769	85.290	83.269	.672	-83.544	-75.192	49.407
400	20.832	89.051	83.936	2.046	-83.636	-73.497	40.156
500	21.844	93.816	85.450	4.183	-83.718	-70.951	31.012
600	22.557	97.865	87.190	6.405	-83.750	-68.394	24.912
700	23.095	101.384	88.971	8.689	-83.747	-65.835	20.554
800	23.518	104.497	90.721	11.021	-83.715	-63.275	17.286
900	23.857	107.287	92.409	13.390	-83.671	-60.724	14.746
1000	24.132	109.815	94.025	15.790	-83.607	-58.169	12.713
1100	24.358	112.126	95.567	18.215	-83.536	-55.636	11.054
1200	24.545	114.254	97.037	20.660	-83.457	-53.104	9.671
1300	24.700	116.225	98.438	23.123	-83.375	-50.578	8.503
1400	24.831	118.060	99.775	25.599	-83.293	-48.053	7.501
1500	24.941	119.777	101.052	28.088	-83.212	-45.551	6.637
1600	25.035	121.390	102.273	30.587	-83.133	-43.044	5.879
1687	25.105	122.717	103.293	32.769	-83.067	-40.846	5.292
1687	25.105	122.717	103.293	32.769	-95.149	-40.846	5.292
1700	25.116	122.910	103.442	33.095	-95.131	-40.423	5.197
1800	25.185	124.348	104.565	35.610	-94.991	-37.207	4.517
1900	25.245	125.711	105.642	38.131	-94.851	-33.997	3.911
2000	25.297	127.007	106.678	40.658	-94.712	-30.806	3.366

*Enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 22.530 + 1.704\times10^{-3}T - 3.396\times10^{5}T^{-2}$
$H° - H°_{298} = 22.530\times10^{-3}T + 0.852\times10^{-6}T^{2} + 3.396\times10^{2}T^{-1} - 7.932$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -69.247 - 13.513\times10^{-3}T + 0.442\times10^{-6}T^{2} + 249.350T^{-1}$
$\Delta Gf° = -69.247 + 13.513\times10^{-3}T\ln T - 0.442\times10^{-6}T^{2} + 124.675T^{-1} - 97.328\times10^{-3}T$
332.6-1687 K: $\Delta Hf° = -84.247 + 0.228\times10^{-3}T + 0.209\times10^{-6}T^{2} + 202.250T^{-1}$
$\Delta Gf° = -84.247 - 0.228\times10^{-3}T\ln T - 0.209\times10^{-6}T^{2} + 101.125T^{-1} + 27.704\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -96.676 - 0.193\times10^{-3}T + 0.560\times10^{-6}T^{2} + 300.750T^{-1}$
$\Delta Gf° = -96.676 + 0.193\times10^{-3}T\ln T - 0.560\times10^{-6}T^{2} + 150.375T^{-1} + 32.519\times10^{-3}T$

Source: Data from Chase (80) who estimated enthalpy of formation at 298 K.

$SiH_2Br_2(g)$
Dibromosilane (ideal gas)

[Formation: $Si(c,l) + H_2(g) + Br_2(l,g) = SiH_2Br_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.665	74.077	74.077	0	-45.500	-46.094	33.787
300	15.710	74.174	74.077	.029	-45.526	-46.097	33.581
332.6	16.355	75.828	74.169	.552	-45.975	-46.136	30.315
332.6	16.355	75.828	74.169	.552	-53.040	-46.136	30.315
400	17.689	78.982	74.720	1.705	-53.293	-44.716	24.431
500	19.092	83.088	75.992	3.548	-53.577	-42.536	18.592
600	20.161	86.667	77.479	5.513	-53.772	-40.309	14.682
700	21.017	89.842	79.023	7.573	-53.898	-38.056	11.881
800	21.717	92.695	80.556	9.711	-53.966	-35.784	9.775
900	22.293	95.288	82.052	11.912	-53.995	-33.511	8.137
1000	22.770	97.662	83.496	14.166	-53.987	-31.227	6.825
1100	23.167	99.851	84.884	16.464	-53.954	-28.959	5.753
1200	23.498	101.882	86.218	18.797	-53.904	-26.689	4.861
1300	23.775	103.774	87.496	21.161	-53.841	-24.425	4.106
1400	24.009	105.544	88.722	23.551	-53.770	-22.158	3.459
1500	24.207	107.208	89.900	25.962	-53.697	-19.915	2.902
1600	24.377	108.776	91.032	28.391	-53.622	-17.668	2.413
1687	24.503	110.070	91.980	30.518	-53.556	-15.693	2.033
1687	24.503	110.070	91.980	30.518	-65.638	-15.693	2.033
1700	24.522	110.258	92.119	30.837	-65.620	-15.303	1.967
1800	24.648	111.663	93.166	33.295	-65.480	-12.346	1.499
1900	24.757	112.999	94.175	35.766	-65.337	-9.395	1.081
2000	24.852	114.271	95.148	38.246	-65.196	-6.462	.706

*Enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:

$$Cp° = 19.395 + 3.392\times10^{-3}T - 4.215\times10^{5}T^{-2}$$

$$H°-H°_{298} = 19.395\times10^{-3}T + 1.696\times10^{-6}T^{2} + 4.215\times10^{2}T^{-1} - 7.347$$

Formation equations (kcal/mol):

298.15-332.6 K:

$$\Delta Hf° = -43.501 - 10.831\times10^{-3}T + 1.026\times10^{-6}T^{2} + 339.500T^{-1}$$

$$\Delta Gf° = -43.501 + 10.831\times10^{-3}T\ln T - 1.026\times10^{-6}T^{2} + 169.750T^{-1} - 72.011\times10^{-3}T$$

332.6-1687 K:

$$\Delta Hf° = -53.501 - 1.670\times10^{-3}T + 0.871\times10^{-6}T^{2} + 308.100T^{-1}$$

$$\Delta Gf° = -53.501 + 1.670\times10^{-3}T\ln T - 0.871\times10^{-6}T^{2} + 154.050T^{-1} + 11.344\times10^{-3}T$$

1687-2000 K:

$$\Delta Hf° = -65.930 - 2.091\times10^{-3}T + 1.222\times10^{-6}T^{2} + 406.600T^{-1}$$

$$\Delta Gf° = -65.930 + 2.091\times10^{-3}T\ln T - 1.222\times10^{-6}T^{2} + 203.300T^{-1} + 16.158\times10^{-3}T$$

Source: Data from Chase (80) who estimated enthalpy of formation at 298 K and some molecular constants.

$SiH_3Br(g)$
Bromosilane (ideal gas)
[Formation: $Si(c,l) + 1.5H_2(g) + 0.5Br_2(l,g) = SiH_3Br(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	12.635	62.704	62.704	0	-18.700	-16.674	12.222
300	12.680	62.782	62.705	.023	-18.722	-16.661	12.138
332.6	13.379	64.126	62.780	.448	-19.088	-16.419	10.788
332.6	13.379	64.126	62.780	.448	-22.620	-16.419	10.788
400	14.823	66.736	63.229	1.403	-23.011	-15.126	8.264
500	16.505	70.231	64.285	2.973	-23.477	-13.097	5.724
600	17.876	73.366	65.543	4.694	-23.822	-10.988	4.002
700	19.019	76.210	66.867	6.540	-24.066	-8.830	2.757
800	19.977	78.814	68.200	8.491	-24.227	-6.639	1.814
900	20.779	81.215	69.515	10.530	-24.324	-4.435	1.077
1000	21.450	83.440	70.797	12.643	-24.366	-2.215	.484
1100	22.010	85.511	72.041	14.817	-24.369	-.006	.001
1200	22.480	87.447	73.245	17.042	-24.343	2.209	-.402
1300	22.875	89.263	74.409	19.310	-24.297	4.418	-.743
1400	23.210	90.970	75.531	21.615	-24.236	6.630	-1.035
1500	23.494	92.582	76.615	23.951	-24.167	8.820	-1.285
1600	23.737	94.106	77.661	26.312	-24.094	11.014	-1.504
1687	23.918	95.367	78.541	28.386	-24.028	12.946	-1.677
1687	23.918	95.367	78.541	28.386	-36.110	12.946	-1.677
1700	23.945	95.551	78.670	28.697	-36.092	13.327	-1.713
1800	24.125	96.925	79.647	31.100	-35.950	16.231	-1.971
1900	24.282	98.234	80.591	33.521	-35.804	19.127	-2.200
2000	24.419	99.483	81.505	35.956	-35.658	22.008	-2.405

*Enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.285 + 5.030 \times 10^{-3}T - 4.577 \times 10^{5}T^{-2}$

$H°- H°_{298} = 16.285 \times 10^{-3}T + 2.515 \times 10^{-6}T^{2} + 4.577 \times 10^{2}T^{-1} - 6.614$

Formation equations (kcal/mol):

298.15-332.6 K: $ΔHf° = -17.707 - 8.123 \times 10^{-3}T + 1.586 \times 10^{-6}T^{2} + 383.950T^{-1}$

$ΔGf° = -17.707 + 8.123 \times 10^{-3}T\ln T - 1.586 \times 10^{-6}T^{2} + 191.975T^{-1} - 44.507 \times 10^{-3}T$

332.6-1687 K: $ΔHf° = -22.707 - 3.543 \times 10^{-3}T + 1.508 \times 10^{-6}T^{2} + 368.250T^{-1}$

$ΔGf° = -22.707 + 3.543 \times 10^{-3}T\ln T - 1.508 \times 10^{-6}T^{2} + 184.125T^{-1} - 2.829 \times 10^{-3}T$

1687-2000 K: $ΔHf° = -35.136 - 3.964 \times 10^{-3}T + 1.859 \times 10^{-6}T^{2} + 466.750T^{-1}$

$ΔGf° = -35.136 + 3.964 \times 10^{-3}T\ln T - 1.859 \times 10^{-6}T^{2} + 233.375T^{-1} + 1.985 \times 10^{-3}T$

Source: Data from Chase (80) who estimated enthalpy of formation at 298 K.

$SiHCl_3(g)$

Trichlorosilane (ideal gas)

[Formation: $Si(c,l) + 0.5H_2(g) + 1.5Cl_2(g) = SiHCl_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.034	74.953	74.953	0	-119.300	-111.821	81.966
300	18.078	75.065	74.955	.033	-119.305	-111.775	81.427
400	19.994	80.549	75.689	1.944	-119.493	-109.236	59.683
500	21.236	85.153	77.133	4.010	-119.602	-106.655	46.618
600	22.099	89.105	78.807	6.179	-119.659	-104.061	37.904
700	22.740	92.562	80.531	8.422	-119.675	-101.461	31.677
800	23.234	95.632	82.230	10.722	-119.662	-98.859	27.007
900	23.625	98.392	83.874	13.066	-119.628	-96.259	23.375
1000	23.939	100.898	85.453	15.445	-119.577	-93.658	20.469
1100	24.195	103.192	86.963	17.852	-119.516	-91.077	18.095
1200	24.406	105.307	88.405	20.282	-119.448	-88.495	16.117
1300	24.580	107.268	89.782	22.732	-119.374	-85.919	14.444
1400	24.726	109.095	91.097	25.197	-119.300	-83.345	13.011
1500	24.849	110.805	92.354	27.676	-119.226	-80.790	11.771
1600	24.953	112.412	93.558	30.166	-119.155	-78.232	10.686
1687	25.031	113.736	94.565	32.341	-119.094	-75.986	9.844
1687	25.031	113.736	94.565	32.341	-131.176	-75.986	9.844
1700	25.043	113.928	94.713	32.666	-131.159	-75.556	9.713
1800	25.119	115.361	95.819	35.175	-131.025	-72.287	8.777
1900	25.186	116.721	96.884	37.690	-130.891	-69.025	7.940
2000	25.243	118.015	97.910	40.211	-130.760	-65.781	7.188

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.935 + 2.134 \times 10^{-3}T - 4.033 \times 10^{5}T^{-2}$

$H° - H°_{298} = 21.935 \times 10^{-3}T + 1.067 \times 10^{-6}T^{2} + 4.033 \times 10^{2}T^{-1} - 7.987$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -119.976 - 0.212 \times 10^{-3}T + 0.374 \times 10^{-6}T^{2} + 210.600T^{-1}$

$\Delta Gf° = -119.976 + 0.212 \times 10^{-3}T\ln T - 0.374 \times 10^{-6}T^{2} + 105.300T^{-1} + 25.070 \times 10^{-3}T$

1687-2000 K: $\Delta Hf° = -132.405 - 0.634 \times 10^{-3}T + 0.725 \times 10^{-6}T^{2} + 309.100T^{-1}$

$\Delta Gf° = -132.405 + 0.634 \times 10^{-3}T\ln T - 0.725 \times 10^{-6}T^{2} + 154.550T^{-1} + 29.884 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Farber (141). Other data from Chase (80).

$SiH_2Cl_2(g)$
Dichlorosilane (ideal gas)
[Formation: $Si(c,l) + H_2(g) + Cl_2(g) = SiH_2Cl_2(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	14.860	68.504	68.504	0	-75.300	-69.190	50.717
300	14.908	68.596	68.504	.028	-75.309	-69.152	50.376
400	17.094	73.203	69.118	1.634	-75.734	-67.034	36.625
500	18.649	77.193	70.343	3.425	-76.041	-64.820	28.332
600	19.823	80.702	71.784	5.351	-76.256	-62.556	22.786
700	20.751	83.830	73.284	7.382	-76.396	-60.261	18.814
800	21.502	86.651	74.781	9.496	-76.479	-57.948	15.830
900	22.116	89.220	76.244	11.678	-76.518	-55.628	13.508
1000	22.622	91.578	77.663	13.915	-76.521	-53.301	11.649
1100	23.041	93.754	79.028	16.199	-76.497	-50.987	10.130
1200	23.390	95.774	80.340	18.521	-76.455	-48.669	8.864
1300	23.681	97.658	81.600	20.875	-76.399	-46.356	7.793
1400	23.927	99.423	82.812	23.256	-76.335	-44.044	6.875
1500	24.135	101.081	83.975	25.659	-76.268	-41.752	6.083
1600	24.313	102.644	85.093	28.082	-76.198	-39.454	5.389
1687	24.445	103.935	86.032	30.203	-76.138	-37.435	4.850
1687	24.445	103.935	86.032	30.203	-88.220	-37.435	4.850
1700	24.465	104.123	86.169	30.521	-88.202	-37.039	4.762
1800	24.596	105.525	87.206	32.974	-88.067	-34.033	4.132
1900	24.710	106.858	88.205	35.440	-87.929	-31.032	3.569
2000	24.810	108.128	89.170	37.916	-87.793	-28.047	3.065

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.086 + 3.570x10^{-3}T - 4.703x10^{5}T^{-2}$
$H° - H°_{298} = 19.086x10^{-3}T + 1.785x10^{-6}T^{2} + 4.703x10^{2}T^{-1} - 7.427$

Formation equations (kcal/mol):

298.15-1687 K: $ΔHf° = -75.896 - 1.876x10^{-3}T + 0.927x10^{-6}T^{2} + 320.000T^{-1}$
$ΔGf° = -75.896 + 1.876x10^{-3}T\ln T - 0.927x10^{-6}T^{2} + 160.000T^{-1} + 10.281x10^{-3}T$
1687-2000 K: $ΔHf° = -88.325 - 2.297x10^{-3}T + 1.278x10^{-6}T^{2} + 418.500T^{-1}$
$ΔGf° = -88.325 + 2.297x10^{-3}T\ln T - 1.278x10^{-6}T^{2} + 209.250T^{-1} + 15.095x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Farber (141). Other data from Chase (80).

$SiH_3Cl(g)$
Chlorosilane (ideal gas)
[Formation: $Si(c,l) + 1.5H_2(g) + 0.5Cl_2(g) = SiH_3Cl(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	12.212	59.906	59.906	0	-32.400	-27.019	19.805
300	12.259	59.982	59.906	.023	-32.413	-26.985	19.658
400	14.498	63.828	60.416	1.365	-33.034	-25.080	13.703
500	16.260	67.260	61.448	2.906	-33.514	-23.032	10.067
600	17.688	70.355	62.678	4.606	-33.871	-20.902	7.613
700	18.872	73.173	63.979	6.436	-34.124	-18.719	5.844
800	19.859	75.760	65.293	8.374	-34.293	-16.505	4.509
900	20.683	78.148	66.590	10.402	-34.396	-14.275	3.466
1000	21.370	80.364	67.858	12.506	-34.444	-12.029	2.629
1100	21.943	82.428	69.090	14.672	-34.453	-9.794	1.946
1200	22.422	84.359	70.283	16.891	-34.432	-7.553	1.376
1300	22.826	86.170	71.436	19.154	-34.389	-5.315	.894
1400	23.166	87.874	72.550	21.454	-34.332	-3.076	.480
1500	23.456	89.483	73.626	23.786	-34.266	-.858	.125
1600	23.703	91.004	74.664	26.144	-34.196	1.365	-.186
1687	23.887	92.265	75.540	28.214	-34.133	3.320	-.430
1687	23.887	92.265	75.540	28.214	-46.215	3.320	-.430
1700	23.915	92.448	75.669	28.525	-46.197	3.706	-.476
1800	24.098	93.820	76.639	30.926	-46.057	6.639	-.806
1900	24.258	95.128	77.579	33.344	-45.914	9.563	-1.100
2000	24.397	96.375	78.487	35.777	-45.771	12.475	-1.363

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.099 + 5.138\times10^{-3}T - 4.817\times10^{5}T^{-2}$

$H°-H°_{298} = 16.099\times10^{-3}T + 2.569\times10^{-6}T^{2} + 4.817\times10^{2}T^{-1} - 6.644$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -32.695 - 3.678\times10^{-3}T + 1.546\times10^{-6}T^{2} + 373.800T^{-1}$

$\Delta Gf° = -32.695 + 3.678\times10^{-3}T\ln T - 1.546\times10^{-6}T^{2} + 186.900T^{-1} - 3.557\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -45.124 - 4.099\times10^{-3}T + 1.897\times10^{-6}T^{2} + 472.300T^{-1}$

$\Delta Gf° = -45.124 + 4.099\times10^{-3}T\ln T - 1.897\times10^{-6}T^{2} + 236.150T^{-1} + 1.257\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Farber (141). Other data from Chase (80).

$SiHF_3(g)$
Trifluorosilane (ideal gas)
[Formation: $Si(c,l) + 0.5H_2(g) + 1.5F_2(g) = SiHF_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	15.173	66.242	66.242	0	-287.000	-279.091	204.577
300	15.224	66.336	66.243	.028	-287.008	-279.043	203.280
400	17.606	71.058	66.870	1.675	-287.369	-276.331	150.978
500	19.340	75.184	68.130	3.527	-287.618	-273.539	119.562
600	20.599	78.827	69.614	5.528	-287.785	-270.708	98.604
700	21.538	82.076	71.166	7.637	-287.889	-267.853	83.626
800	22.257	85.001	72.716	9.828	-287.949	-264.985	72.390
900	22.817	87.656	74.230	12.083	-287.977	-262.111	63.648
1000	23.263	90.084	75.696	14.388	-287.978	-259.230	56.654
1100	23.621	92.319	77.108	16.732	-287.964	-256.364	50.934
1200	23.913	94.387	78.462	19.110	-287.934	-253.492	46.167
1300	24.153	96.311	79.763	21.513	-287.897	-250.623	42.133
1400	24.352	98.108	81.009	23.939	-287.855	-247.754	38.676
1500	24.520	99.794	82.205	26.383	-287.813	-244.902	35.682
1600	24.661	101.381	83.355	28.842	-287.769	-242.044	33.061
1687	24.765	102.690	84.319	30.992	-287.732	-239.537	31.031
1687	24.765	102.690	84.319	30.992	-299.814	-239.537	31.031
1700	24.781	102.880	84.460	31.314	-299.799	-239.068	30.734
1800	24.885	104.300	85.523	33.798	-299.692	-235.498	28.593
1900	24.974	105.647	86.546	36.291	-299.582	-231.931	26.678
2000	25.051	106.930	87.534	38.792	-299.474	-228.381	24.956

*Enthalpy of formation at 298 K estimated.

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 20.483 + 2.856\times10^{-3}T - 5.478\times10^{5}T^{-2}$

$H°- H°_{298} = 20.483\times10^{-3}T + 1.428\times10^{-6}T^{2} + 5.478\times10^{2}T^{-1} - 8.071$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -287.729 - 1.186\times10^{-3}T + 0.607\times10^{-6}T^{2} + 306.800T^{-1}$

$\Delta Gf° = -287.729 + 1.186\times10^{-3}T\ln T - 0.607\times10^{-6}T^{2} + 153.400T^{-1} + 20.670\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -300.158 - 1.607\times10^{-3}T + 0.957\times10^{-6}T^{2} + 405.300T^{-1}$

$\Delta Gf° = -300.158 + 1.607\times10^{-3}T\ln T - 0.957\times10^{-6}T^{2} + 202.650T^{-1} + 25.484\times10^{-3}T$

Source: Data from Chase (82) who estimated enthalpy of formation at 298 K.

$SiH_2F_2(g)$
Difluorosilane (ideal gas)
[Formation: $Si(c,l) + H_2(g) + F_2(g) = SiH_2F_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	12.970	62.624	62.624	0	-189.000	-182.582	133.835
300	13.021	62.704	62.624	.024	-189.012	-182.542	132.980
400	15.467	66.799	63.167	1.453	-189.553	-180.302	98.511
500	17.346	70.461	64.265	3.098	-189.957	-177.938	77.776
600	18.788	73.757	65.577	4.908	-190.249	-175.507	63.928
700	19.921	76.742	66.963	6.845	-190.453	-173.034	54.023
800	20.826	79.463	68.358	8.884	-190.587	-170.534	46.587
900	21.558	81.960	69.732	11.005	-190.668	-168.021	40.801
1000	21.155	84.263	71.071	13.192	-190.707	-165.495	36.168
1100	22.644	86.398	72.369	15.432	-190.716	-162.981	32.381
1200	23.049	88.386	73.621	17.718	-190.701	-160.459	29.223
1300	23.386	90.245	74.830	20.040	-190.670	-157.940	26.552
1400	23.669	91.989	75.994	22.393	-190.630	-155.421	24.262
1500	23.908	93.630	77.115	24.772	-190.584	-152.919	22.280
1600	24.111	95.180	78.196	27.174	-190.533	-150.411	20.545
1687	24.262	96.461	79.105	29.278	-190.488	-148.208	19.200
1687	24.262	96.461	79.105	29.278	-202.570	-148.208	19.200
1700	24.285	96.647	79.239	29.594	-202.555	-147.784	18.999
1800	24.435	98.039	80.245	32.030	-202.438	-144.564	17.552
1900	24.564	99.364	81.217	34.480	-202.317	-141.352	16.259
2000	24.677	100.627	82.156	36.942	-202.197	-138.153	15.096

*Enthalpy of formation at 298 K estimated.

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 17.996 + 4.104\times10^{-3}T - 5.555\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.996\times10^{-3}T + 2.052\times10^{-6}T^2 + 5.555\times10^{2}T^{-1} - 7.411$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf^\circ = -189.560 - 2.647\times10^{-3}T + 1.108\times10^{-6}T^2 + 373.000T^{-1}$

$\Delta Gf^\circ = -189.560 + 2.647\times10^{-3}T\ln T - 1.108\times10^{-6}T^2 + 186.500T^{-1} + 6.556\times10^{-3}T$

1687-2000 K: $\Delta Hf^\circ = -201.989 - 3.068\times10^{-3}T + 1.459\times10^{-6}T^2 + 471.500T^{-1}$

$\Delta Gf^\circ = -201.989 + 3.068\times10^{-3}T\ln T - 1.459\times10^{-6}T^2 + 235.750T^{-1} + 11.370\times10^{-3}T$

Source: Data from Chase (82) who estimated enthalpy of formation at 298 K.

$SiH_3F(g)$
Fluorosilane (ideal gas)
[Formation: $Si(c,l) + 1.5H_2(g) + 0.5F_2(g) = SiH_3F(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.280	56.952	56.952	0	-90.000	-84.460	61.910
300	11.326	57.022	56.952	.021	-90.014	-84.426	61.504
400	13.668	60.611	57.426	1.274	-90.694	-82.458	45.052
500	15.590	63.875	58.395	2.740	-91.225	-80.334	35.114
600	17.156	66.860	59.560	4.380	-91.622	-78.118	28.454
700	18.447	69.605	60.802	6.162	-91.908	-75.845	23.679
800	19.516	72.140	62.063	8.062	-92.103	-73.533	20.088
900	20.401	74.492	63.315	10.059	-92.228	-71.205	17.291
1000	21.135	76.680	64.543	12.137	-92.295	-68.857	15.048
1100	21.745	78.724	65.740	14.282	-92.319	-66.519	13.216
1200	22.253	80.639	66.903	16.483	-92.311	-64.173	11.687
1300	22.680	82.437	68.029	18.730	-92.281	-61.829	10.394
1400	23.039	84.132	69.120	21.017	-92.235	-59.486	9.286
1500	23.344	85.732	70.175	23.336	-92.181	-57.160	8.328
1600	23.604	87.247	71.195	25.684	-92.119	-54.829	7.489
1687	23.798	88.502	72.055	27.746	-92.064	-52.780	6.838
1687	23.798	88.502	72.055	27.746	-104.146	-52.780	6.838
1700	23.827	88.685	72.181	28.056	-104.129	-52.380	6.734
1800	24.020	90.052	73.136	30.448	-103.998	-49.338	5.990
1900	24.187	91.355	74.061	32.859	-103.863	-46.303	5.326
2000	24.332	92.600	74.957	35.285	-103.728	-43.285	4.730

*Enthalpy of formation at 298 K estimated.

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 15.434 + 5.530\times10^{-3}T - 5.158\times10^{5}T^{-2}$
$H°- H°_{298} = 15.434\times10^{-3}T + 2.765\times10^{-6}T^{2} + 5.158\times10^{2}T^{-1} - 6.577$

Formation equations (kcal/mol):

298.15-1687 K: $ΔHf° = -90.218 - 4.183\times10^{-3}T + 1.699\times10^{-6}T^{2} + 391.800T^{-1}$
$ΔGf° = -90.218 + 4.183\times10^{-3}T\ln T - 1.699\times10^{-6}T^{2} + 195.900T^{-1} - 6.219\times10^{-3}T$
1687-2000 K: $ΔHf° = -102.647 - 4.604\times10^{-3}T + 2.050\times10^{-6}T^{2} + 490.300T^{-1}$
$ΔGf° = -102.647 + 4.604\times10^{-3}T\ln T - 2.050\times10^{-6}T^{2} + 245.150T^{-1} - 1.405\times10^{-3}T$

Source: Data from Chase (82) who estimated enthalpy of formation at 298 K.

$SiHI_3(g)$
Triiodosilane (ideal gas)
[Formation: $Si(c,l) + 0.5H_2(g) + 1.5I_2(c,l,g) = SiHI_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	20.049	89.602	89.602	0	-17.800	-26.107	19.137
300	20.081	89.726	89.603	.037	-17.814	-26.158	19.056
386.8	21.247	94.987	90.239	1.836	-18.566	-28.479	16.091
386.8	21.247	94.987	90.239	1.836	-24.129	-28.479	16.091
400	21.424	95.703	90.408	2.118	-24.345	-28.624	15.639
458.4	21.925	98.662	91.274	3.386	-25.284	-29.179	13.911
458.4	21.925	98.662	91.274	3.386	-40.315	-29.179	13.911
500	22.282	100.582	91.970	4.306	-40.330	-28.165	12.311
600	22.894	104.701	93.758	6.566	-40.338	-25.733	9.373
700	23.364	108.267	95.581	8.880	-40.314	-23.301	7.275
800	23.738	111.412	97.367	11.236	-40.267	-20.870	5.701
900	24.041	114.226	99.087	13.625	-40.210	-18.450	4.480
1000	24.289	116.773	100.731	16.042	-40.138	-16.028	3.503
1100	24.493	119.097	102.295	18.482	-40.058	-13.628	2.708
1200	24.662	121.236	103.786	20.940	-39.976	-11.229	2.045
1300	24.803	123.216	105.206	23.413	-39.889	-8.837	1.486
1400	24.921	125.058	106.559	25.899	-39.806	-6.447	1.006
1500	25.021	126.781	107.850	28.397	-39.724	-4.079	.594
1600	25.107	128.399	109.085	30.903	-39.646	-1.706	.233
1687	25.171	129.730	110.115	33.091	-39.581	.377	-.049
1687	25.171	129.730	110.115	33.091	-51.663	.377	-.049
1700	25.180	129.923	110.265	33.418	-51.645	.782	-.101
1800	25.243	131.364	111.398	35.939	-51.508	3.864	-.469
1900	25.297	132.731	112.486	38.466	-51.373	6.936	-.798
2000	25.345	134.029	113.530	40.998	-51.238	9.997	-1.092

*Enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 22.751 + 1.626\times10^{-3}T - 2.833\times10^{5}T^{-2}$
$H° - H°_{298} = 22.751\times10^{-3}T + 0.813\times10^{-6}T^2 + 2.833\times10^{2}T^{-1} - 7.806$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -16.640 - 5.471\times10^{-3}T - 1.985\times10^{-6}T^2 + 193.050T^{-1}$
$\Delta Gf° = -16.640 + 5.471\times10^{-3}T\ln T + 1.985\times10^{-6}T^2 + 96.525T^{-1} - 64.605\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -18.822 - 15.078\times10^{-3}T + 0.253\times10^{-6}T^2 + 193.050T^{-1}$
$\Delta Gf° = -18.822 + 15.078\times10^{-3}T\ln T - 0.253\times10^{-6}T^2 + 96.525T^{-1} - 115.328\times10^{-3}T$
458.4-1687 K: $\Delta Hf° = -40.892 + 0.433\times10^{-3}T + 0.151\times10^{-6}T^2 + 170.100T^{-1}$
$\Delta Gf° = -40.892 - 0.433\times10^{-3}T\ln T - 0.151\times10^{-6}T^2 + 85.050T^{-1} + 27.866\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -53.321 + 0.011\times10^{-3}T + 0.502\times10^{-6}T^2 + 268.600T^{-1}$
$\Delta Gf° = -53.321 - 0.011\times10^{-3}T\ln T - 0.502\times10^{-6}T^2 + 134.300T^{-1} + 32.680\times10^{-3}T$

Source: Data from Chase (80) who estimated enthalpy of formation at 298 K and some molecular constants.

$SiH_2I_2(g)$
Diiodosilane (ideal gas)
[Formation: $Si(c,l) + H_2(g) + I_2(c,l,g) = SiH_2I_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.247	78.079	78.079	0	-9.100	-13.457	9.864
300	16.289	78.180	78.080	.030	-9.116	-13.484	9.823
386.8	17.884	82.530	78.602	1.519	-9.874	-14.651	8.278
386.8	17.884	82.530	78.602	1.519	-13.583	-14.651	8.278
400	18.126	83.134	78.742	1.757	-13.762	-14.684	8.023
458.4	18.881	85.662	79.465	2.840	-14.527	-14.762	7.038
458.4	18.881	85.662	79.465	2.840	-24.548	-14.762	7.038
500	19.419	87.325	80.051	3.637	-24.645	-13.868	6.062
600	20.410	90.957	81.572	5.631	-24.820	-11.697	4.260
700	21.211	94.165	83.146	7.713	-24.930	-9.501	2.966
800	21.872	97.042	84.707	9.868	-24.987	-7.289	1.991
900	22.419	99.651	86.224	12.084	-25.006	-5.076	1.233
1000	22.875	102.037	87.688	14.349	-24.992	-2.854	.624
1100	23.255	104.236	89.094	16.656	-24.955	-.651	.129
1200	23.572	106.273	90.441	18.998	-24.902	1.558	-.284
1300	23.839	108.171	91.733	21.369	-24.836	3.760	-.632
1400	24.065	109.946	92.972	23.764	-24.766	5.961	-.931
1500	24.257	111.613	94.159	26.181	-24.692	8.141	-1.186
1600	24.420	113.184	95.300	28.615	-24.617	10.327	-1.411
1687	24.543	114.481	96.256	30.745	-24.554	12.247	-1.587
1687	24.543	114.481	96.256	30.745	-36.636	12.247	-1.587
1700	24.561	114.669	96.396	31.064	-36.618	12.628	-1.623
1800	24.682	116.076	97.450	33.526	-36.480	15.522	-1.885
1900	24.788	117.413	98.466	36.000	-36.341	18.409	-2.118
2000	24.880	118.687	99.445	38.483	-36.203	21.281	-2.325

*Enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.630 + 3.254\times10^{-3}T - 3.870\times10^{5}T^{-2}$
$H°-H°_{298} = 19.630\times10^{-3}T + 1.627\times10^{-6}T^{2} + 3.870\times10^{2}T^{-1} - 7.295$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -8.462 - 5.382\times10^{-3}T - 0.635\times10^{-6}T^{2} + 305.000T^{-1}$
$\Delta Gf° = -8.462 + 5.382\times10^{-3}T\ln T + 0.635\times10^{-6}T^{2} + 152.500T^{-1} - 49.324\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -9.917 - 11.786\times10^{-3}T + 0.857\times10^{-6}T^{2} + 305.000T^{-1}$
$\Delta Gf° = -9.917 + 11.786\times10^{-3}T\ln T - 0.857\times10^{-6}T^{2} + 152.500T^{-1} - 83.139\times10^{-3}T$
458.4-1687 K: $\Delta Hf° = -24.630 - 1.446\times10^{-3}T + 0.789\times10^{-6}T^{2} + 289.700T^{-1}$
$\Delta Gf° = -24.630 + 1.446\times10^{-3}T\ln T - 0.789\times10^{-6}T^{2} + 144.850T^{-1} + 12.324\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -37.059 - 1.867\times10^{-3}T + 1.140\times10^{-6}T^{2} + 388.200T^{-1}$
$\Delta Gf° = -37.059 + 1.867\times10^{-3}T\ln T - 1.140\times10^{-6}T^{2} + 194.100T^{-1} + 17.138\times10^{-3}T$

Source: Data from Chase (80) who estimated enthalpy of formation at 298 K and some molecular constants.

$SiH_3I(g)$
Iodosilane (ideal gas)
[Formation: $Si(c,l) + 1.5H_2(g) + 0.5I_2(c,l,g) = SiH_3I(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.002	64.749	64.749	0	-.500	-.369	.270
300	13.045	64.829	64.749	.024	-.516	-.368	.268
386.8	14.836	68.375	65.173	1.238	-1.247	-.229	.129
386.8	14.836	68.375	65.173	1.238	-3.101	-.229	.129
400	15.108	68.877	65.287	1.436	-3.239	-.129	.070
458.4	16.052	71.005	65.881	2.349	-3.815	.369	-.176
458.4	16.052	71.005	65.881	2.349	-8.826	.369	-.176
500	16.725	72.429	66.367	3.031	-8.997	1.211	-.529
600	18.048	75.599	67.646	4.772	-9.327	3.284	-1.196
700	19.157	78.467	68.991	6.633	-9.559	5.404	-1.687
800	20.089	81.087	70.341	8.597	-9.709	7.556	-2.064
900	20.872	83.500	71.671	10.646	-9.799	9.719	-2.360
1000	21.528	85.734	72.967	12.767	-9.836	11.898	-2.600
1100	22.077	87.813	74.224	14.948	-9.834	14.063	-2.794
1200	22.538	89.754	75.437	17.180	-9.805	16.236	-2.957
1300	22.926	91.574	76.610	19.453	-9.755	18.403	-3.094
1400	23.254	93.285	77.740	21.763	-9.692	20.572	-3.211
1500	23.533	94.899	78.830	24.103	-9.622	22.720	-3.310
1600	23.771	96.426	79.884	26.468	-9.547	24.870	-3.397
1687	23.949	97.689	80.769	28.544	-9.482	26.764	-3.467
1687	23.949	97.689	80.769	28.544	-21.564	26.764	-3.467
1700	23.976	97.873	80.899	28.856	-21.545	27.140	-3.489
1800	24.153	99.249	81.881	31.262	-21.403	30.000	-3.642
1900	24.307	100.559	82.830	33.686	-21.258	32.854	-3.779
2000	24.442	101.809	83.747	36.123	-21.113	35.692	-3.900

*Enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.459 + 4.930\times10^{-3}T - 4.380\times10^{5}T^{-2}$
$H°- H°_{298} = 16.459\times10^{-3}T + 2.465\times10^{-6}T^{2} + 4.380\times10^{2}T^{-1} - 6.595$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -0.195 - 5.343\times10^{-3}T + 0.739\times10^{-6}T^{2} + 364.250T^{-1}$
$\Delta Gf° = -0.195 + 5.343\times10^{-3}T\ln T - 0.739\times10^{-6}T^{2} + 182.125T^{-1} - 32.852\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -0.922 - 8.545\times10^{-3}T + 1.485\times10^{-6}T^{2} + 364.250T^{-1}$
$\Delta Gf° = -0.922 + 8.545\times10^{-3}T\ln T - 1.485\times10^{-6}T^{2} + 182.125T^{-1} - 49.759\times10^{-3}T$
458.4-1687 K: $\Delta Hf° = -8.279 - 3.375\times10^{-3}T + 1.451\times10^{-6}T^{2} + 356.600T^{-1}$
$\Delta Gf° = -8.279 + 3.375\times10^{-3}T\ln T - 1.451\times10^{-6}T^{2} + 178.300T^{-1} - 2.028\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -20.708 - 3.796\times10^{-3}T + 1.802\times10^{-6}T^{2} + 455.100T^{-1}$
$\Delta Gf° = -20.708 + 3.796\times10^{-3}T\ln T - 1.802\times10^{-6}T^{2} + 227.550T^{-1} + 2.786\times10^{-3}T$

Source: Data from Chase (80) who estimated enthalpy of formation at 298 K.

$SiN(g)$
Silicon Mononitride (ideal gas)
[Formation: $Si(c,l) + 0.5N_2(g) = SiN(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.210	51.792	51.792	0	89.000	81.723	-59.904
300	7.216	51.837	51.794	.013	88.997	81.677	-59.501
400	7.541	53.957	52.080	.751	88.880	79.253	-43.301
500	7.843	55.673	52.631	1.521	88.753	76.863	-33.596
600	8.086	57.125	53.262	2.318	88.621	74.496	-27.135
700	8.273	58.387	53.907	3.136	88.485	72.151	-22.526
800	8.421	59.501	54.537	3.971	88.343	69.829	-19.076
900	8.545	60.501	55.147	4.819	88.191	67.523	-16.397
1000	8.657	61.407	55.727	5.680	88.037	65.244	-14.259
1100	8.767	62.237	56.282	6.551	87.877	62.965	-12.510
1200	8.880	63.005	56.811	7.433	87.715	60.706	-11.056
1300	8.999	63.720	57.315	8.327	87.554	58.463	-9.828
1400	9.123	64.392	57.797	9.233	87.392	56.234	-8.778
1500	9.253	65.025	58.257	10.152	87.233	54.005	-7.868
1600	9.384	65.627	58.700	11.084	87.079	51.792	-7.074
1687	9.499	66.127	59.070	11.905	86.948	49.897	-6.464
1687	9.499	66.127	59.070	11.905	74.866	49.897	-6.464
1700	9.516	66.200	59.124	12.029	74.856	49.709	-6.390
1800	9.645	66.747	59.532	12.987	74.780	48.235	-5.857
1900	9.770	67.272	59.926	13.958	74.715	46.763	-5.379
2000	9.888	67.776	60.306	14.941	74.659	45.287	-4.949

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.489 + 1.204\times10^{-3}T - 0.567\times10^{5}T^{-2}$
$H°- H°_{298} = 7.489\times10^{-3}T + 0.602\times10^{-6}T^{2} + 0.567\times10^{2}T^{-1} - 2.477$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = 89.563 - 1.448\times10^{-3}T - 0.043\times10^{-6}T^{2} - 37.850T^{-1}$
$\Delta Gf° = 89.563 + 1.448\times10^{-3}T\ln T + 0.043\times10^{-6}T^{2} - 18.925T^{-1} - 34.347\times10^{-3}T$
1687-2000 K: $\Delta Hf° = 77.134 - 1.870\times10^{-3}T + 0.307\times10^{-6}T^{2} + 60.650T^{-1}$
$\Delta Gf° = 77.134 + 1.870\times10^{-3}T\ln T - 0.307\times10^{-6}T^{2} + 30.325T^{-1} - 29.533\times10^{-3}T$

Source: Data from JANAF (127).

$Si_2N(g)$
Disilicon Nitride (ideal gas)
[Formation: $2Si(c,l) + 0.5N_2(g) = Si_2N(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.922	61.275	61.275	0	95.000	86.237	-63.213
300	11.942	61.349	61.276	.022	94.998	86.183	-62.783
400	12.803	64.910	61.755	1.262	94.875	83.259	-45.490
500	13.374	67.833	62.687	2.573	94.743	80.373	-35.130
600	13.755	70.307	63.755	3.931	94.600	77.509	-28.232
700	14.017	72.449	64.849	5.320	94.443	74.671	-23.313
800	14.202	74.333	65.918	6.732	94.274	71.863	-19.632
900	14.336	76.014	66.948	8.159	94.082	69.072	-16.773
1000	14.435	77.530	67.932	9.598	93.877	66.321	-14.494
1100	14.512	78.909	68.868	11.045	93.656	63.561	-12.628
1200	14.571	80.175	69.759	12.499	93.422	60.833	-11.079
1300	14.618	81.343	70.605	13.959	93.176	58.128	-9.772
1400	14.656	82.428	71.412	15.423	92.916	55.450	-8.656
1500	14.687	83.440	72.180	16.890	92.643	52.761	-7.687
1600	14.712	84.389	72.914	18.360	92.358	50.107	-6.844
1687	14.730	85.168	73.526	19.640	92.100	47.859	-6.200
1687	14.730	85.168	73.526	19.640	67.936	47.859	-6.200
1700	14.733	85.281	73.615	19.832	67.915	47.713	-6.134
1800	14.751	86.124	74.287	21.306	67.745	46.534	-5.650
1900	14.767	86.922	74.931	22.782	67.575	45.361	-5.218
2000	14.780	87.680	75.550	24.260	67.404	44.185	-4.828

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.918 + 0.600\times10^{-3}T - 1.933\times10^{5}T^{-2}$

$H°- H°_{298} = 13.918\times10^{-3}T + 0.300\times10^{-6}T^{2} + 1.933\times10^{2}T^{-1} - 4.825$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = 95.269 - 0.698\times10^{-3}T - 0.697\times10^{-6}T^{2} + 0.250T^{-1}$

$\Delta Gf° = 95.269 + 0.698\times10^{-3}T\ln T + 0.697\times10^{-6}T^{2} + 0.125T^{-1} - 34.482\times10^{-3}T$

1687-2000 K: $\Delta Hf° = 70.411 - 1.540\times10^{-3}T + 0.005\times10^{-6}T^{2} + 197.250T^{-1}$

$\Delta Gf° = 70.411 + 1.540\times10^{-3}T\ln T - 0.005\times10^{-6}T^{2} + 98.625T^{-1} - 24.854\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$Si_3N_4(\alpha)$
α-Trisilicon Tetranitride
[Formation: $3Si(c,l) + 2N_2(g) = Si_3N_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.230	15.790	15.790	0	-188.300	-161.690	118.521
300	22.339	15.928	15.791	.041	-188.312	-161.526	117.670
400	26.675	23.008	16.726	2.513	-188.755	-152.528	83.336
500	29.412	29.272	18.622	5.325	-188.987	-143.437	62.695
600	31.471	34.824	20.869	8.373	-189.081	-134.321	48.926
700	33.168	39.806	23.225	11.607	-189.074	-125.195	39.087
800	34.639	44.333	25.584	14.999	-188.983	-116.069	31.708
900	35.948	48.490	27.901	18.530	-188.830	-106.962	25.974
1000	37.132	52.340	30.155	22.185	-188.609	-97.853	21.385
1100	38.214	55.930	32.336	25.953	-188.328	-88.813	17.645
1200	39.208	59.299	34.445	29.825	-187.988	-79.783	14.530
1300	40.124	62.473	36.479	33.792	-187.593	-70.779	11.899
1400	40.971	65.478	38.444	37.847	-187.151	-61.798	9.647
1500	41.755	68.332	40.343	41.984	-186.661	-52.894	7.707
1600	42.482	71.051	42.179	46.196	-186.125	-44.002	6.010
1687	43.069	73.315	43.725	49.919	-185.627	-36.221	4.692
1687	43.069	73.315	43.725	49.919	-221.873	-36.221	4.692
1700	43.157	73.646	43.952	50.479	-221.769	-34.779	4.471
1800	43.784	76.131	45.672	54.826	-220.948	-23.796	2.889
1900	44.368	78.514	47.338	59.234	-220.076	-12.866	1.480
2000	44.913	80.804	48.955	63.698	-219.158	-2.002	.219

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 28.119 + 9.364\times10^{-3}T - 7.717\times10^{5}T^{-2}$
$H°- H°_{298} = 28.119\times10^{-3}T + 4.682\times10^{-6}T^{2} + 7.717\times10^{2}T^{-1} - 11.388$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -189.586 - 1.952\times10^{-3}T + 2.451\times10^{-6}T^{2} + 492.000T^{-1}$
$\Delta Gf° = -189.586 + 1.952\times10^{-3}T\ln T - 2.451\times10^{-6}T^{2} + 246.000T^{-1} + 80.405\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -226.873 - 3.215\times10^{-3}T + 3.504\times10^{-6}T^{2} + 787.500T^{-1}$
$\Delta Gf° = -226.873 + 3.215\times10^{-3}T\ln T - 3.504\times10^{-6}T^{2} + 393.750T^{-1} + 94.847\times10^{-3}T$

Source: Data from Gurvich (195).

$SiOF_2(g)$
Silicon Oxide Difluoride (ideal gas)
[Formation: $Si(c,l) + 0.5O_2(g) + F_2(g) = SiOF_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	12.832	64.806	64.806	0	-231.000	-227.232	166.563
300	12.871	64.885	64.806	.024	-231.005	-227.208	165.519
400	14.656	68.847	65.335	1.405	-231.256	-225.904	123.427
500	15.922	72.261	66.385	2.938	-231.438	-224.542	98.146
600	16.818	75.248	67.620	4.577	-231.579	-223.151	81.282
700	17.462	77.891	68.901	6.293	-231.691	-221.737	69.229
800	17.932	80.255	70.175	8.064	-231.786	-220.308	60.185
900	18.284	82.389	71.417	9.875	-231.872	-218.868	53.148
1000	18.551	84.330	72.612	11.718	-231.951	-217.411	47.515
1100	18.758	86.108	73.759	13.584	-232.027	-215.960	42.907
1200	18.921	87.747	74.857	15.468	-232.102	-214.496	39.065
1300	19.052	89.267	75.908	17.367	-232.176	-213.026	35.812
1400	19.158	90.683	76.914	19.277	-232.256	-211.547	33.024
1500	19.245	92.008	77.876	21.198	-232.336	-210.076	30.608
1600	19.317	93.252	78.798	23.126	-232.420	-208.590	28.492
1687	19.370	94.276	79.570	24.809	-232.496	-207.271	26.851
1687	19.370	94.276	79.570	24.809	-244.578	-207.271	26.851
1700	19.378	94.425	79.683	25.061	-244.581	-206.979	26.609
1800	19.429	95.534	80.533	27.001	-244.607	-204.764	24.861
1900	19.473	96.586	81.351	28.946	-244.632	-202.550	23.298
2000	19.511	97.586	82.138	30.896	-244.659	-200.340	21.892

*Data estimated.

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.814 + 1.824 \times 10^{-3}T - 4.023 \times 10^{5}T^{-2}$

$H° - H°_{298} = 16.814 \times 10^{-3}T + 0.912 \times 10^{-6}T^{2} + 4.023 \times 10^{2}T^{-1} - 6.443$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -231.324 - 0.988 \times 10^{-3}T + 0.135 \times 10^{-6}T^{2} + 180.700T^{-1}$

$\Delta Gf° = -231.324 + 0.988 \times 10^{-3}T\ln T - 0.135 \times 10^{-6}T^{2} + 90.350T^{-1} + 7.119 \times 10^{-3}T$

1687-2000 K: $\Delta Hf° = -243.753 - 1.409 \times 10^{-3}T + 0.487 \times 10^{-6}T^{2} + 279.200T^{-1}$

$\Delta Gf° = -243.753 + 1.409 \times 10^{-3}T\ln T - 0.487 \times 10^{-6}T^{2} + 139.600T^{-1} + 11.933 \times 10^{-3}T$

Source: Data are those estimated by JANAF (127).

$Si_2ON_2(c)$
Silicon Oxynitride
[Formation: $2Si(c,l) + 0.5O_2(g) + N_2(g) = Si_2ON_2(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	15.670	10.580	10.580	0	-226.500	-206.019	151.014
300	15.770	10.680	10.580	.030	-226.508	-205.892	149.990
400	21.530	16.210	11.310	1.960	-226.643	-198.998	108.726
500	24.030	21.310	12.810	4.250	-226.514	-192.096	83.964
600	25.510	25.830	14.597	6.740	-226.258	-185.228	67.469
700	26.530	29.850	16.507	9.340	-225.956	-178.424	55.706
800	27.280	33.440	18.402	12.030	-225.618	-171.652	46.893
900	27.900	36.690	20.257	14.790	-225.265	-164.927	40.049
1000	28.410	39.660	22.050	17.610	-224.889	-158.226	34.580
1100	28.880	42.390	23.772	20.480	-224.501	-151.588	30.117
1200	29.290	44.920	25.437	23.380	-224.113	-144.986	26.405
1300	29.690	47.280	27.026	26.330	-223.701	-138.407	23.268
1400	30.060	49.490	28.547	29.320	-223.279	-131.845	20.582
1500	30.410	51.580	30.020	32.340	-222.849	-125.361	18.265
1600	30.750	53.550	31.425	35.400	-222.399	-118.873	16.237
1687	31.046	55.182	32.605	38.086	-222.001	-113.207	14.666
1687	31.046	55.182	32.605	38.086	-246.165	-113.207	14.666
1700	31.090	55.420	32.779	38.490	-246.087	-112.175	14.421
1800	31.410	57.210	34.088	41.620	-245.469	-104.311	12.665
1900	31.740	58.920	35.352	44.780	-244.829	-96.489	11.099
2000	32.050	60.560	36.575	47.970	-244.167	-88.718	9.695

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 27.074 + 2.554\times10^{-3}T - 10.815\times10^{5}T^{-2}$
$H°-H°_{298} = 27.074\times10^{-3}T + 1.277\times10^{-6}T^{2} + 10.815\times10^{2}T^{-1} - 11.813$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -231.059 + 5.584\times10^{-3}T - 0.266\times10^{-6}T^{2} + 869.800T^{-1}$
$\Delta Gf° = -231.059 - 5.584\times10^{-3}T\ln T + 0.266\times10^{-6}T^{2} + 434.900T^{-1} + 110.826\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -255.917 + 4.742\times10^{-3}T + 0.436\times10^{-6}T^{2} + 1066.800T^{-1}$
$\Delta Gf° = -255.917 - 4.742\times10^{-3}T\ln T - 0.436\times10^{-6}T^{2} + 533.400T^{-1} + 120.454\times10^{-3}T$

Sources: Heat capacity and entropy at 298 K from Koshchenko (283). Other data from Fegley (145).

SiSe(g)
Silicon Monoselenide (ideal gas)
[Reaction: $Si(c,l) + 0.5Se_2(g) = SiSe(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	8.030	56.200	56.200	0	31.850	25.112	-18.407
300	8.040	56.250	56.203	.014	31.846	25.069	-18.263
400	8.390	58.620	56.520	.840	31.667	22.836	-12.477
500	8.550	60.510	57.134	1.688	31.465	20.653	-9.027
600	8.650	62.080	57.833	2.548	31.248	18.507	-6.741
700	8.710	63.420	58.540	3.416	31.020	16.401	-5.120
800	8.750	64.590	59.229	4.289	30.784	14.328	-3.914
900	8.780	65.620	59.880	5.166	30.539	12.287	-2.984
1000	8.810	66.550	60.504	6.046	30.292	10.276	-2.246
1100	8.830	67.390	61.092	6.928	30.040	8.282	-1.645
1200	8.850	68.160	61.649	7.813	29.786	6.314	-1.150
1300	8.870	68.870	62.178	8.699	29.531	4.369	-.735
1400	8.880	69.520	62.673	9.586	29.273	2.456	-.383
1500	8.900	70.140	63.156	10.476	29.014	.529	-.077
1600	8.910	70.710	63.606	11.366	28.754	-1.358	.186
1687	8.927	71.181	63.984	12.142	28.526	-2.961	.384
1687	8.927	71.181	63.984	12.142	16.444	-2.961	.384
1700	8.930	71.250	64.039	12.258	16.419	-3.105	.399
1800	8.940	71.760	64.454	13.151	16.225	-4.250	.516
1900	8.950	72.250	64.857	14.046	16.037	-5.395	.621
2000	8.960	72.710	65.239	14.942	15.853	-6.527	.713

ase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.781 + 0.100\times10^{-3}T - 0.690\times10^{5}T^{-2}$

$H°- H°_{298} = 8.781\times10^{-3}T + 0.050\times10^{-6}T^{2} + 0.690\times10^{2}T^{-1} - 2.854$

Reaction equations (kcal/mol):

298.15-1687 K: $ΔHr° = 32.727 - 2.230\times10^{-3}T - 0.141\times10^{-6}T^{2} - 59.450T^{-1}$

$ΔGr° = 32.727 + 2.230\times10^{-3}T\ln T + 0.141\times10^{-6}T^{2} - 29.725T^{-1} - 37.954\times10^{-3}T$

1687-2000 K: $ΔHr° = 20.298 - 2.651\times10^{-3}T + 0.209\times10^{-6}T^{2} + 39.050T^{-1}$

$ΔGr° = 20.298 + 2.651\times10^{-3}T\ln T - 0.209\times10^{-6}T^{2} + 19.525T^{-1} - 33.140\times10^{-3}T$

Source: Data from Mills (332).

SiTe(g)
Silicon Monotelluride (ideal gas)
[Reaction: Si(c,l) + 0.5Te_2(g) = SiTe(g)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15	8.250	58.200	58.200	0	33.335	26.548	-19.460
300	8.260	58.250	58.200	.015	33.333	26.505	-19.309
400	8.530	60.670	58.528	.857	33.228	24.242	-13.245
500	8.660	62.590	59.156	1.717	33.094	22.012	-9.621
600	8.730	64.180	59.868	2.587	32.936	19.808	-7.215
700	8.780	65.530	60.583	3.463	32.757	17.633	-5.505
800	8.810	66.700	61.271	4.343	32.558	15.490	-4.232
900	8.840	67.740	61.934	5.225	32.340	13.368	-3.246
1000	8.860	68.670	62.560	6.110	32.108	11.283	-2.466
1100	8.870	69.520	63.160	6.996	31.860	9.200	-1.828
1200	8.880	70.290	63.720	7.884	31.599	7.155	-1.303
1300	8.900	71.000	64.252	8.773	31.326	5.131	-.863
1400	8.910	71.660	64.758	9.663	31.038	3.129	-.489
1500	8.920	72.280	65.244	10.554	30.744	1.127	-.164
1600	8.920	72.850	65.696	11.446	30.446	-.834	.114
1687	8.929	73.321	66.076	12.223	30.184	-2.498	.324
1687	8.929	73.321	66.076	12.223	18.102	-2.498	.324
1700	8.930	73.390	66.132	12.339	18.071	-2.652	.341
1800	8.940	73.910	66.558	13.233	17.835	-3.882	.471
1900	8.950	74.390	66.955	14.127	17.602	-5.074	.584
2000	8.960	74.850	67.339	15.022	17.372	-6.268	.685

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.851 + 0.060\times10^{-3}T - 0.550\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.851\times10^{-3}T + 0.030\times10^{-6}T^2 + 0.550\times10^{2}T^{-1} - 2.826$

Reaction equations (kcal/mol):

298.15-1687 K: $\Delta Hr^\circ = 33.913 - 1.128\times10^{-3}T - 0.617\times10^{-6}T^2 - 55.600T^{-1}$

$\Delta Gr^\circ = 33.913 + 1.128\times10^{-3}T\ln T + 0.617\times10^{-6}T^2 - 27.800T^{-1} - 30.997\times10^{-3}T$

1687-2000 K: $\Delta Hr^\circ = 21.483 - 1.548\times10^{-3}T - 0.266\times10^{-6}T^2 + 42.900T^{-1}$

$\Delta Gr^\circ = 21.483 + 1.548\times10^{-3}T\ln T + 0.266\times10^{-6}T^2 + 21.450T^{-1} - 26.183\times10^{-3}T$

Source: Data from Mills (332).

$SmC_2(c)$
Samarium Dicarbide
[Formation: $Sm(c,l) + 2C(c) = SmC_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.680	21.010	21.010	0	-23.000	-23.488	17.217
300	16.710	21.110	21.010	.030	-22.991	-23.492	17.114
400	17.990	26.120	21.695	1.770	-22.485	-23.743	12.972
500	18.700	30.210	22.990	3.610	-22.125	-24.093	10.531
600	19.200	33.670	24.487	5.510	-21.916	-24.509	8.927
700	19.590	36.660	26.017	7.450	-21.826	-24.947	7.789
800	19.920	39.300	27.525	9.420	-21.807	-25.401	6.939
900	20.220	41.660	28.960	11.430	-21.833	-25.845	6.276
1000	20.510	43.810	30.340	13.470	-21.878	-26.288	5.745
1100	20.780	45.770	31.652	15.530	-21.966	-26.709	5.307
1190	21.014	47.414	32.784	17.410	-22.075	-27.116	4.980
1190	21.014	47.414	32.784	17.410	-22.819	-27.116	4.980
1200	21.040	47.590	32.907	17.620	-22.829	-27.142	4.943
1300	21.290	49.290	34.105	19.740	-22.931	-27.512	4.625
1345	21.403	50.016	34.626	20.701	-22.976	-27.660	4.494
1345	21.403	50.016	34.626	20.701	-25.036	-27.660	4.494
1400	21.540	50.870	35.241	21.880	-25.134	-27.760	4.334
1440	21.640	51.480	35.687	22.740	-25.206	-27.838	4.225
1440	21.640	52.400	35.687	24.070	-23.876	-27.838	4.225
1500	21.790	53.290	36.370	25.380	-23.970	-27.993	4.079
1600	22.030	54.710	37.479	27.570	-24.128	-28.272	3.862
1700	22.270	56.050	38.532	29.780	-24.282	-28.525	3.667
1800	22.510	57.330	39.541	32.020	-24.416	-28.779	3.494
1900	22.750	58.550	40.503	34.290	-24.530	-29.003	3.336
2000	22.990	59.730	41.445	36.570	-24.646	-29.246	3.196

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1190 K, α − β transition point of Sm; ΔH° = 0.744 kcal/mol.
1345 K, melting point of Sm; ΔH° = 2.060 kcal/mol.
1440 K, α − β transition point of SmC_2; ΔH° = 1.330 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1440 K: $Cp° = 18.444 + 2.274 \times 10^{-3}T - 2.171 \times 10^{5}T^{-2}$
$H° - H°_{298} = 18.444 \times 10^{-3}T + 1.137 \times 10^{-6}T^{2} + 2.171 \times 10^{2}T^{-1} - 6.328$
1440-2000 K: $Cp° = 23.053 + 0.418 \times 10^{-3}T - 41.790 \times 10^{5}T^{-2}$
$H° - H°_{298} = 23.053 \times 10^{-3}T + 0.209 \times 10^{-6}T^{2} + 41.790 \times 10^{2}T^{-1} - 12.462$

Formation equations (kcal/mol):

298.15-1190 K: $\Delta Hf° = -22.758 + 3.208 \times 10^{-3}T - 1.880 \times 10^{-6}T^{2} - 307.500T^{-1}$
$\Delta Gf° = -22.758 - 3.208 \times 10^{-3}T\ln T + 1.880 \times 10^{-6}T^{2} - 153.750T^{-1} + 16.999 \times 10^{-3}T$
1190-1345 K: $\Delta Hf° = -22.162 + 0.188 \times 10^{-3}T - 0.395 \times 10^{-6}T^{2} - 127.500T^{-1}$
$\Delta Gf° = -22.162 - 0.188 \times 10^{-3}T\ln T + 0.395 \times 10^{-6}T^{2} - 63.750T^{-1} - 3.184 \times 10^{-3}T$
1345-1440 K: $\Delta Hf° = -23.173 - 0.592 \times 10^{-3}T - 0.395 \times 10^{-6}T^{2} - 127.500T^{-1}$
$\Delta Gf° = -23.173 + 0.592 \times 10^{-3}T\ln T + 0.395 \times 10^{-6}T^{2} - 63.750T^{-1} - 8.052 \times 10^{-3}T$
1440-2000 K: $\Delta Hf° = -29.307 + 4.017 \times 10^{-3}T - 1.323 \times 10^{-6}T^{2} + 3834.400T^{-1}$
$\Delta Gf° = -29.307 - 4.017 \times 10^{-3}T\ln T + 1.323 \times 10^{-6}T^{2} + 1917.200T^{-1} + 27.434 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Haschke (201). Other data based on their estimates.

$SmFeO_3(c)$
Samarium Ferrite
[Formation: $Sm(c) + Fe(c) + 1.5O_2(g) = SmFeO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	25.660	25.000	25.000	0	-325.030	-303.665	222.590
300	25.690	25.160	25.000	.050	-325.023	-303.531	221.120
400	27.600	32.810	26.035	2.710	-324.801	-296.405	161.946
500	29.650	39.180	28.020	5.580	-324.555	-289.318	126.459
600	31.760	44.780	30.363	8.650	-324.292	-282.303	102.827
700	33.880	49.830	32.787	11.930	-323.975	-275.322	85.958
800	36.030	54.500	35.225	15.420	-323.580	-268.409	73.325
900	38.180	58.860	37.604	19.130	-323.116	-261.533	63.508
1000	40.330	63.000	39.940	23.060	-322.633	-254.718	55.668

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 18.600 + 21.680x10^{-3}T + 0.530x10^{5}T^{-2}$

$H°- H°_{298} = 18.600x10^{-3}T + 10.840x10^{-6}T^{2} - 0.530x10^{2}T^{-1} - 6.331$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -324.946 - 0.224x10^{-3}T + 2.529x10^{-6}T^{2} - 72.300T^{-1}$

$\Delta Gf° = -324.946 + 0.224x10^{-3}T\ln T - 2.529x10^{-6}T^{2} - 36.150T^{-1} + 71.259x10^{-3}T$

Source: Data based on Kaul (237).

$SmN(c)$
Samarium Nitride
[Formation: $Sm(c,l) + 0.5N_2(g) = SmN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	11.700	17.600	17.600	0	-77.000	-70.466	51.652
300	11.710	17.670	17.603	.020	-77.000	-70.428	51.306
400	11.840	21.060	18.060	1.200	-76.914	-68.250	37.290
500	11.980	23.720	18.940	2.390	-76.922	-66.085	28.885
600	12.110	25.910	19.927	3.590	-77.015	-63.916	23.281
700	12.240	27.790	20.919	4.810	-77.160	-61.716	19.268
800	12.380	29.430	21.880	6.040	-77.335	-59.496	16.253
900	12.520	30.900	22.800	7.290	-77.526	-57.253	13.903
1000	12.650	32.220	23.670	8.550	-77.725	-54.981	12.016
1100	12.780	33.430	24.503	9.820	-77.949	-52.705	10.471
1190	12.906	34.442	25.223	10.971	-78.179	-50.637	9.300
1190	12.906	34.442	25.223	10.971	-78.923	-50.637	9.300
1200	12.920	34.550	25.300	11.100	-78.946	-50.389	9.177
1300	13.060	35.590	26.052	12.400	-79.174	-48.009	8.071
1345	13.118	36.035	26.378	12.989	-79.274	-46.919	7.624
1345	13.118	36.035	26.378	12.989	-81.334	-46.919	7.624
1400	13.190	36.560	26.767	13.710	-81.499	-45.510	7.104
1500	13.320	37.480	27.453	15.040	-81.784	-42.930	6.255
1600	13.460	38.340	28.103	16.380	-82.062	-40.330	5.509
1700	13.600	39.160	28.731	17.730	-82.333	-37.712	4.848
1800	13.730	39.940	29.329	19.100	-82.587	-35.085	4.260
1900	13.870	40.690	29.911	20.480	-82.834	-32.445	3.732
2000	14.000	41.400	30.465	21.870	-83.073	-29.772	3.253

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1190 K, α - β transition point of Sm; ΔH° = 0.744 kcal/mol.
1345 K, melting point of Sm; ΔH° = 2.060 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.300 + 1.350\times10^{-3}T$
$H°-H°_{298} = 11.300\times10^{-3}T + 0.675\times10^{-6}T^2 - 3.429$

Formation equations (kcal/mol):

298.15-1190 K: $\Delta Hf° = -76.264 - 0.158\times10^{-3}T - 1.105\times10^{-6}T^2 - 176.050T^{-1}$
$\Delta Gf° = -76.264 + 0.158\times10^{-3}T\ln T + 1.105\times10^{-6}T^2 - 88.025T^{-1} + 19.205\times10^{-3}T$
1190-1345 K: $\Delta Hf° = -75.668 - 3.179\times10^{-3}T + 0.381\times10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf° = -75.668 + 3.179\times10^{-3}T\ln T - 0.381\times10^{-6}T^2 + 1.975T^{-1} - 0.979\times10^{-3}T$
1345-2000 K: $\Delta Hf° = -76.679 - 3.958\times10^{-3}T + 0.381\times10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf° = -76.679 + 3.958\times10^{-3}T\ln T - 0.381\times10^{-6}T^2 + 1.975T^{-1} - 5.847\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Brown (60). Other data are those estimated by Brown (59).

$SmO(g)$
Samarium Monoxide (ideal gas)
[Formation: $Sm(c,l) + 0.5O_2(g) = SmO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.560	61.299	61.299	0	-28.000	-34.013	24.932
300	7.560	61.346	61.299	.014	-28.006	-34.051	24.806
400	7.940	63.576	61.601	.790	-28.330	-36.019	19.680
500	8.220	65.380	62.182	1.599	-28.733	-37.893	16.563
600	8.400	66.895	62.845	2.430	-29.216	-39.684	14.455
700	8.520	68.199	63.518	3.277	-29.760	-41.381	12.920
800	8.610	69.343	64.177	4.133	-30.337	-43.003	11.748
900	8.670	70.361	64.808	4.998	-30.941	-44.550	10.818
1000	8.720	71.277	65.410	5.867	-31.556	-46.028	10.059
1100	8.760	72.110	65.982	6.741	-32.201	-47.453	9.428
1190	8.778	72.800	66.472	7.530	-32.815	-48.676	8.939
1190	8.778	72.800	66.472	7.530	-33.559	-48.676	8.939
1200	8.780	72.873	66.525	7.618	-33.625	-48.792	8.886
1300	8.810	73.577	67.040	8.498	-34.296	-50.039	8.412
1345	8.814	73.877	67.264	8.895	-34.598	-50.569	8.217
1345	8.814	73.877	67.264	8.895	-36.658	-50.569	8.217
1400	8.820	74.230	67.531	9.379	-37.072	-51.132	7.982
1500	8.840	74.840	67.998	10.263	-37.823	-52.108	7.592
1600	8.850	75.411	68.444	11.147	-38.577	-53.043	7.245
1700	8.860	75.948	68.870	12.033	-39.332	-53.920	6.932
1800	8.870	76.454	69.277	12.919	-40.090	-54.765	6.649
1900	8.880	76.934	69.667	13.807	-40.849	-55.558	6.391
2000	8.880	77.390	70.043	14.695	-41.611	-56.305	6.153

Phase changes: 1190 K, α - β transition point of Sm; ΔH° = 0.744 kcal/mol.
1345 K, melting point of Sm; ΔH° = 2.060 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.447 + 0.302\text{x}10^{-3}T - 0.869\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 8.447\text{x}10^{-3}T + 0.151\text{x}10^{-6}T^{2} + 0.869\text{x}10^{2}T^{-1} - 2.823$

Formation equations (kcal/mol):

298.15-1190 K: $\Delta Hf° = -26.467 - 3.368\text{x}10^{-3}T - 1.586\text{x}10^{-6}T^{2} - 115.700T^{-1}$
$\Delta Gf° = -26.467 + 3.368\text{x}10^{-3}T\ln T + 1.586\text{x}10^{-6}T^{2} - 57.850T^{-1} - 44.320\text{x}10^{-3}T$
1190-1345 K: $\Delta Hf° = -25.871 - 6.388\text{x}10^{-3}T - 0.100\text{x}10^{-6}T^{2} + 64.300T^{-1}$
$\Delta Gf° = -25.871 + 6.388\text{x}10^{-3}T\ln T + 0.100\text{x}10^{-6}T^{2} + 32.150T^{-1} - 64.504\text{x}10^{-3}T$
1345-2000 K: $\Delta Hf° = -26.882 - 7.168\text{x}10^{-3}T - 0.100\text{x}10^{-6}T^{2} + 64.300T^{-1}$
$\Delta Gf° = -26.882 + 7.168\text{x}10^{-3}T\ln T + 0.100\text{x}10^{-6}T^{2} + 32.150T^{-1} - 69.372\text{x}10^{-3}T$

Source: Data from Pedley (396).

Sm_6WO_{12}(c)
Hexasamarium Tungstate
[Formation: $6Sm(c,l) + W(c) + 6O_2(g) = Sm_6WO_{12}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	95.720	121.350	121.350	0	-1559.000	-1475.440	1081.513
300	96.070	121.940	121.350	.180	-1558.987	-1474.923	1074.467
400	109.300	151.610	125.310	10.520	-1557.974	-1447.042	790.617
500	116.880	176.870	133.150	21.860	-1556.702	-1419.429	620.424
600	122.230	198.680	142.313	33.820	-1555.512	-1392.125	507.075
700	126.520	217.850	151.750	46.270	-1554.368	-1364.944	426.149
800	130.260	234.990	161.103	59.110	-1553.146	-1337.970	365.512
900	133.670	250.540	170.196	72.310	-1551.843	-1311.152	318.387
1000	136.880	264.790	178.950	85.840	-1550.346	-1284.476	280.718
1100	139.960	277.980	187.362	99.680	-1548.793	-1258.008	249.940
1190	142.651	289.095	194.640	112.402	-1547.369	-1234.276	226.678
1190	142.651	289.095	194.640	112.402	-1551.833	-1234.276	226.678
1200	142.950	290.290	195.432	113.830	-1551.655	-1231.545	224.292
1300	145.870	301.840	203.171	128.270	-1549.752	-1204.995	202.575
1345	147.166	306.826	206.556	134.863	-1548.819	-1193.018	193.852
1345	147.166	306.826	206.556	134.863	-1561.179	-1193.018	193.852
1400	148.750	312.760	210.617	143.000	-1560.235	-1177.996	183.891
1500	151.600	323.120	217.773	158.020	-1558.321	-1150.744	167.661

Phase changes: 1190 K, α – β transition point of Sm; ΔH° = 0.744 kcal/mol.
1345 K, melting point of Sm; ΔH° = 2.060 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15–1500 K: $Cp° = 112.036 + 27.016\times10^{-3}T - 21.666\times10^{5}T^{-2}$
$H°-H°_{298} = 112.036\times10^{-3}T + 13.508\times10^{-6}T^{2} + 21.666\times10^{2}T^{-1} - 41.871$

Formation equations (kcal/mol):

298.15–1190 K: $\Delta Hf° = -1565.839 + 13.641\times10^{-3}T + 1.209\times10^{-6}T^{2} + 794.400T^{-1}$
$\Delta Gf° = -1565.839 - 13.641\times10^{-3}T\ln T - 1.209\times10^{-6}T^{2} + 397.200T^{-1} + 376.811\times10^{-3}T$
1190–1345 K: $\Delta Hf° = -1562.265 - 4.479\times10^{-3}T + 10.119\times10^{-6}T^{2} + 1874.400T^{-1}$
$\Delta Gf° = -1562.265 + 4.479\times10^{-3}T\ln T - 10.119\times10^{-6}T^{2} + 937.200T^{-1} + 255.709\times10^{-3}T$
1345–1500 K: $\Delta Hf° = -1568.330 - 9.159\times10^{-3}T + 10.119\times10^{-6}T^{2} + 1874.400T^{-1}$
$\Delta Gf° = -1568.330 + 9.159\times10^{-3}T\ln T - 10.119\times10^{-6}T^{2} + 937.200T^{-1} + 226.503\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Levitskii (303). Other data based on Nadiradze (345).

$SnH_4(g)$
Tin Tetrahydride (ideal gas), Stannane
[Formation: $Sn(\beta,l) + 2H_2(g) = SnH_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	12.090	54.650	54.650	0	38.900	44.863	-32.885
300	12.130	54.730	54.663	.020	38.882	44.896	-32.706
400	14.290	58.520	55.145	1.350	38.157	47.024	-25.692
500	16.070	61.910	56.170	2.870	37.568	49.308	-21.552
505.12	16.147	62.074	56.229	2.952	37.541	49.427	-21.385
505.12	16.147	62.074	56.229	2.952	35.861	49.427	-21.385
600	17.570	64.970	57.387	4.550	35.474	52.015	-18.946
700	18.840	67.780	58.680	6.370	35.206	54.790	-17.106
800	19.900	70.370	59.983	8.310	35.054	57.599	-15.735
900	20.780	72.760	61.260	10.350	34.992	60.431	-14.675
1000	21.480	74.990	62.530	12.460	34.986	63.250	-13.823

Phase change: 505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 12.091 + 10.108\times10^{-3}T - 2.680\times10^{5}T^{-2}$
$H°-H°_{298} = 12.091\times10^{-3}T + 5.054\times10^{-6}T^{2} + 2.680\times10^{2}T^{-1} - 4.953$

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf° = 39.424 - 5.789\times10^{-3}T + 1.874\times10^{-6}T^{2} + 308.600T^{-1}$
$\Delta Gf° = 39.424 + 5.789\times10^{-3}T\ln T - 1.874\times10^{-6}T^{2} + 154.300T^{-1} - 15.919\times10^{-3}T$
505.12-1000 K: $\Delta Hf° = 37.459 - 7.012\times10^{-3}T + 4.035\times10^{-6}T^{2} + 486.400T^{-1}$
$\Delta Gf° = 37.459 + 7.012\times10^{-3}T\ln T - 4.035\times10^{-6}T^{2} + 243.200T^{-1} - 18.898\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Other data based on Shabur (441).

SnO(g)
Tin Monoxide (ideal gas)
[Formation: Sn(β,l) + 0.5O_2(g) = SnO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	7.580	55.446	55.446	0	4.500	-1.078	.790
300	7.590	55.493	55.446	.014	4.496	-1.112	.810
400	7.980	57.734	55.749	.794	4.253	-2.944	1.609
500	8.250	59.544	56.332	1.606	3.989	-4.714	2.060
505.12	8.260	59.628	56.365	1.648	3.974	-4.804	2.079
505.12	8.260	59.628	56.365	1.648	2.294	-4.804	2.079
600	8.440	61.066	56.998	2.441	2.072	-6.114	2.227
700	8.570	62.378	57.675	3.292	1.851	-7.460	2.329
800	8.660	63.528	58.337	4.153	1.633	-8.776	2.398
900	8.730	64.552	58.971	5.023	1.415	-10.064	2.444
1000	8.780	65.474	59.576	5.898	1.197	-11.328	2.476
1100	8.820	66.313	60.151	6.778	.977	-12.570	2.497
1200	8.850	67.082	60.697	7.662	.758	-13.791	2.512
1300	8.880	67.792	61.216	8.549	.536	-14.995	2.521
1400	8.900	68.451	61.710	9.438	.313	-16.181	2.526
1500	8.920	69.066	62.180	10.329	.090	-17.352	2.528
1600	8.940	69.643	62.629	11.223	-.135	-18.509	2.528
1700	8.960	70.186	63.058	12.118	-.361	-19.651	2.526
1800	8.970	70.699	63.468	13.015	-.588	-20.779	2.523
1900	8.990	71.184	63.861	13.913	-.817	-21.893	2.518
2000	9.000	71.645	64.239	14.812	-1.048	-22.997	2.513

Phase change: 505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.466 + 0.348\times10^{-3}T - 0.879\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.466\times10^{-3}T + 0.174\times10^{-6}T^{2} + 0.879\times10^{2}T^{-1} - 2.834$

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf^\circ = 4.505 - 0.117\times10^{-3}T - 2.420\times10^{-6}T^{2} + 72.900T^{-1}$

$\Delta Gf^\circ = 4.505 + 0.117\times10^{-3}T\ln T + 2.420\times10^{-6}T^{2} + 36.450T^{-1} - 20.524\times10^{-3}T$

505.12-2000 K: $\Delta Hf^\circ = 2.540 - 1.340\times10^{-3}T - 0.258\times10^{-6}T^{2} + 250.700T^{-1}$

$\Delta Gf^\circ = 2.540 + 1.340\times10^{-3}T\ln T + 0.258\times10^{-6}T^{2} + 125.350T^{-1} - 23.502\times10^{-3}T$

Source: Data from Pedley (396).

SnSe(c,l)
Tin Selenide
[Reaction: $Sn(\beta,l) + 0.5Se_2(g) = SnSe(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	12.370	20.400	20.400	0	-37.250	-31.008	22.729
300	12.380	20.480	20.413	.020	-37.251	-30.973	22.564
400	12.780	24.100	20.900	1.280	-37.156	-28.894	15.787
500	13.120	26.990	21.830	2.580	-37.070	-26.834	11.729
505.12	13.136	27.124	21.883	2.647	-37.067	-26.730	11.565
505.12	13.136	27.124	21.883	2.647	-38.747	-26.730	11.565
600*	13.430	29.400	22.900	3.900	-38.630	-24.483	8.918
700	13.720	31.500	23.986	5.260	-38.459	-22.139	6.912
800	14.010	33.350	25.036	6.650	-38.253	-19.814	5.413
800	10.130	33.660	25.036	6.900	-38.003	-19.814	5.413
900	11.700	34.960	26.071	8.000	-38.085	-17.540	4.259
1000	12.440	36.230	27.020	9.210	-38.055	-15.256	3.334
1100	12.970	37.440	27.913	10.480	-37.962	-12.978	2.579
1135	13.220	37.850	28.212	10.940	-37.913	-12.183	2.346
1135	22.400	45.120	28.212	19.190	-29.663	-12.183	2.346
1200	22.400	46.370	29.162	20.650	-28.965	-11.201	2.040
1300	22.400	48.160	30.552	22.890	-27.897	-9.758	1.640

*Data extrapolated 580-800 K. Transition at 800 K not well defined.

Phase changes: 505.12 K, melting point of Sn; $\Delta H^\circ = 1.680$ kcal/mol.
800 K, $\alpha - \beta$ transition point of SnSe; $\Delta H^\circ = 0.250$ kcal/mol.
1135 K, melting point of SnSe; $\Delta H^\circ = 8.250$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $C_p^\circ = 11.607 + 3.104\times10^{-3}T - 0.144\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 11.607\times10^{-3}T + 1.552\times10^{-6}T^2 + 0.144\times10^{2}T^{-1} - 3.647$
800-1135 K: $C_p^\circ = 28.055 - 8.326\times10^{-3}T - 72.080\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 28.055\times10^{-3}T - 4.163\times10^{-6}T^2 + 72.080\times10^{2}T^{-1} - 21.890$
1135-1300 K: $C_p^\circ = 22.400$
$H^\circ - H^\circ_{298} = 22.400\times10^{-3}T - 6.234$

Reaction equations (kcal/mol):

298.15-505.12 K: $\Delta Hr^\circ = -37.557 + 1.307\times10^{-3}T - 0.631\times10^{-6}T^2 - 7.950T^{-1}$
$\Delta Gr^\circ = -37.557 - 1.307\times10^{-3}T\ln T + 0.631\times10^{-6}T^2 - 3.975T^{-1} + 29.269\times10^{-3}T$
505.12-800 K: $\Delta Hr^\circ = -39.523 + 0.084\times10^{-3}T + 1.530\times10^{-6}T^2 + 169.850T^{-1}$
$\Delta Gr^\circ = -39.523 - 0.084\times10^{-3}T\ln T - 1.530\times10^{-6}T^2 + 84.925T^{-1} + 26.291\times10^{-3}T$
800-1135 K: $\Delta Hr^\circ = -57.765 + 16.532\times10^{-3}T - 4.184\times10^{-6}T^2 + 7363.450T^{-1}$
$\Delta Gr^\circ = -57.765 - 16.532\times10^{-3}T\ln T + 4.184\times10^{-6}T^2 + 3681.725T^{-1} + 148.851\times10^{-3}T$
1135-1300 K: $\Delta Hr^\circ = -42.109 + 10.877\times10^{-3}T - 0.021\times10^{-6}T^2 + 155.450T^{-1}$
$\Delta Gr^\circ = -42.109 - 10.877\times10^{-3}T\ln T + 0.021\times10^{-6}T^2 + 77.725T^{-1} + 102.800\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wiedemeier (533). Low-temperature heat capacities and entropy at 298 K from Wiedemeier (534) who extrapolated heat capacities 0-230 K to derive entropy at 298 K. High-temperature data based on Wiedemeier (534) and Balde (17). Data extrapolated 580-800 K. Transition at 800 K not well defined.

SnSe(g)
Tin Selenide (ideal gas)
[Reaction: $Sn(\beta,l) + 0.5Se_2(g) = SnSe(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	8.580	60.800	60.800	0	13.650	7.847	-5.752
300	8.590	60.850	60.800	.016	13.645	7.812	-5.691
400	8.740	63.350	61.140	.884	13.348	5.910	-3.229
500	8.810	65.310	61.788	1.761	13.011	4.087	-1.786
505.12	8.812	65.400	61.824	1.806	12.992	3.994	-1.728
505.12	8.812	65.400	61.824	1.806	11.312	3.994	-1.728
600	8.840	66.920	62.513	2.644	11.014	2.649	-.965
700	8.870	68.280	63.237	3.530	10.711	1.285	-.401
800	8.880	69.470	63.949	4.417	10.414	-.044	.012
900	8.890	70.510	64.614	5.306	10.121	-1.329	.323
1000	8.900	71.450	65.255	6.195	9.830	-2.590	.566
1100	8.900	72.300	65.858	7.086	9.544	-3.818	.759
1200	8.910	73.080	66.433	7.976	9.261	-5.027	.915
1300	8.910	73.790	66.969	8.867	8.980	-6.200	1.042
1400	8.910	74.450	67.480	9.758	8.702	-7.358	1.149
1500	8.920	75.060	67.960	10.650	8.429	-8.488	1.237
1600	8.920	75.640	68.426	11.542	8.159	-9.618	1.314
1700	8.920	76.180	68.866	12.434	7.891	-10.712	1.377
1800	8.920	76.690	69.287	13.326	7.626	-11.803	1.433
1900	8.920	77.170	69.687	14.218	7.365	-12.872	1.481
2000	8.920	77.630	70.075	15.110	7.107	-13.939	1.523

Phase change: 505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.931 - 0.310\times10^{5}T^{-2}$
$H°- H°_{298} = 8.931\times10^{-3}T + 0.310\times10^{2}T^{-1} - 2.767$

Reaction equations (kcal/mol):

298.15-505.12 K: $\Delta Hr° = 14.223 - 1.369\times10^{-3}T - 2.183\times10^{-6}T^{2} + 8.650T^{-1}$
$\Delta Gr° = 14.223 + 1.369\times10^{-3}T\ln T + 2.183\times10^{-6}T^{2} + 4.325T^{-1} - 29.886\times10^{-3}T$
505.12-2000 K: $\Delta Hr° = 12.258 - 2.592\times10^{-3}T - 0.021\times10^{-6}T^{2} + 186.450T^{-1}$
$\Delta Gr° = 12.258 + 2.592\times10^{-3}T\ln T + 0.021\times10^{-6}T^{2} + 93.225T^{-1} - 32.864\times10^{-3}T$

Source: Data from Mills (332).

$SnSe_2(c)$
Tin Diselenide
[Reaction: $Sn(\beta,l) + Se_2(g) = SnSe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	17.840	26.700	26.700	0	-61.300	-48.260	35.375
300	17.860	26.810	26.710	.030	-61.300	-48.182	35.100
400	18.350	32.020	27.420	1.840	-61.152	-43.834	23.950
500	18.730	36.160	28.760	3.700	-61.011	-39.517	17.273
505.12	18.747	36.351	28.836	3.796	-61.005	-39.298	17.003
505.12	18.747	36.351	28.836	3.796	-62.685	-39.298	17.003
600*	19.060	39.600	30.283	5.590	-62.506	-34.916	12.718
700	19.370	42.560	31.831	7.510	-62.280	-30.333	9.470

*Data extrapolated above 550 K.

Phase change: 505.12 K, melting point of S_n; ΔH° = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 17.541 + 2.748x10^{-3}T - 0.459x10^{5}T^{-2}$
$H°- H°_{298} = 17.541x10^{-3}T + 1.374x10^{-6}T^{2} + 0.459x10^{2}T^{-1} - 5.506$

Reaction equations (kcal/mol):

298.15-505.12 K: $\Delta Hr° = -61.790 + 1.909x10^{-3}T - 0.649x10^{-6}T^{2} - 6.400T^{-1}$
$\Delta Gr° = -61.790 - 1.909x10^{-3}T\ln T + 0.649x10^{-6}T^{2} - 3.200T^{-1} + 56.099x10^{-3}T$
505.12-700 K: $\Delta Hr° = -63.756 + 0.686x10^{-3}T + 1.512x10^{-6}T^{2} + 171.400T^{-1}$
$\Delta Gr° = -63.756 - 0.686x10^{-3}T\ln T - 1.512x10^{-6}T^{2} + 85.700T^{-1} + 53.120x10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K based on Wiedemeier (533). High-temperature data based on Wiedemeier (534). Data extrapolated above 550 K.

SnTe(c,l)
Tin Telluride
[Reaction: $Sn(\beta,l) + 0.5Te_2(g) = SnTe(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	−(G°− H°₂₉₈)/T	H°− H°₂₉₈	ΔHr°	ΔGr°	
298.15*	11.612	24.000	24.000	0	−33.965	−28.249	20.707
300	11.622	24.072	24.002	.021	−33.964	−28.215	20.554
400	12.149	27.489	24.462	1.211	−33.881	−26.309	14.374
500	12.606	30.251	25.353	2.449	−33.802	−24.426	10.676
505.12	12.626	30.380	25.403	2.514	−33.798	−24.331	10.527
505.12	12.626	30.380	25.403	2.514	−35.478	−24.331	10.527
600	12.991	32.584	26.369	3.729	−35.352	−22.242	8.102
700	13.306	34.611	27.404	5.045	−35.185	−20.069	6.266
800	13.551	36.405	28.420	6.388	−34.995	−17.925	4.897
900	13.724	38.012	29.398	7.753	−34.790	−15.804	3.838
1000	13.827	39.464	30.333	9.131	−34.581	−13.706	2.995
1068	13.857	40.374	30.943	10.072	−34.439	−12.289	2.515
1068	14.876	49.461	30.943	19.777	−24.734	−12.289	2.515
1100	14.876	49.900	31.488	20.253	−24.636	−11.917	2.368
1200	14.876	51.195	33.077	21.741	−24.333	−10.774	1.962

*Entropy at 298 K estimated.

Phase changes: 505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.
1068 K, melting point of SnTe; ΔH° = 9.705 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15−1068 K: $Cp° = 11.848 + 2.170\text{x}10^{-3}T - 0.786\text{x}10^{5}T^{-2}$
$H°- H°_{298} = 11.848\text{x}10^{-3}T + 1.085\text{x}10^{-6}T^{2} + 0.786\text{x}10^{2}T^{-1} - 3.893$
1068−1200 K: $Cp° = 14.876$
$H°- H°_{298} = 14.876\text{x}10^{-3}T + 3.889$

Reaction equations (kcal/mol):

298.15−505.12 K: $\Delta Hr° = -34.845 + 2.580\text{x}10^{-3}T - 1.554\text{x}10^{-6}T^{2} + 74.100T^{-1}$
$\Delta Gr° = -34.845 - 2.580\text{x}10^{-3}T\ln T + 1.554\text{x}10^{-6}T^{2} + 37.050T^{-1} + 35.945\text{x}10^{-3}T$
505.12−1068 K: $\Delta Hr° = -36.810 + 1.357\text{x}10^{-3}T + 0.608\text{x}10^{-6}T^{2} + 251.900T^{-1}$
$\Delta Gr° = -36.810 - 1.357\text{x}10^{-3}T\ln T - 0.608\text{x}10^{-6}T^{2} + 125.950T^{-1} + 32.966\text{x}10^{-3}T$
1068−1200 K: $\Delta Hr° = -29.028 + 4.386\text{x}10^{-3}T - 0.478\text{x}10^{-6}T^{2} + 173.300T^{-1}$
$\Delta Gr° = -29.028 - 4.386\text{x}10^{-3}T\ln T + 0.478\text{x}10^{-6}T^{2} + 86.650T^{-1} + 45.671\text{x}10^{-3}T$

Sources: Enthalpy of formation and estimated entropy at 298 K from Mills (332). High-temperature data based on Medzhidov (328).

SnTe(g)
Tin Telluride (ideal gas)
[Reaction: Sn(b,l) + 0.5Te_2(g) = SnTe(g)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15	8.690	62.700	62.700	0	19.135	13.312	-9.758
300	8.700	62.750	62.700	.016	19.131	13.277	-9.672
400	8.800	65.280	63.048	.893	18.901	11.357	-6.205
500	8.850	67.250	63.698	1.776	18.625	9.502	-4.153
505.12	8.852	67.340	63.734	1.821	18.610	9.407	-4.070
505.12	8.852	67.340	63.734	1.821	16.930	9.407	-4.070
600	8.880	68.860	64.423	2.662	16.681	8.025	-2.923
700	8.900	70.230	65.157	3.551	16.421	6.603	-2.062
800	8.910	71.420	65.869	4.441	16.159	5.216	-1.425
900	8.910	72.470	66.546	5.332	15.889	3.863	-.938
1000	8.920	73.410	67.186	6.224	15.612	2.541	-.555
1100	8.920	74.260	67.791	7.116	15.327	1.250	-.248
1200	8.920	75.040	68.367	8.008	15.034	-.021	.004
1300	8.930	75.750	68.904	8.900	14.734	-1.259	.212
1400	8.930	76.410	69.415	9.793	14.426	-2.474	.386
1500	8.930	77.030	69.906	10.686	14.117	-3.677	.536
1600	8.930	77.610	70.373	11.579	13.808	-4.864	.664
1700	8.930	78.150	70.814	12.472	13.500	-6.013	.773
1800	8.930	78.660	71.234	13.366	13.194	-7.153	.868
1900	8.930	79.140	71.635	14.259	12.890	-8.268	.951
2000	8.930	79.600	72.023	15.153	12.589	-9.377	1.025

Phase change: 505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.940 - 0.217\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.940\times10^{-3}T + 0.217\times10^{2}T^{-1} - 2.738$

Reaction equations (kcal/mol):

298.15-505.12 K: $\Delta Hr^\circ = 19.409 - 0.328\times10^{-3}T - 2.638\times10^{-6}T^{2} + 17.200T^{-1}$

$\Delta Gr^\circ = 19.409 + 0.328\times10^{-3}T\ln T + 2.638\times10^{-6}T^{2} + 8.600T^{-1} - 23.199\times10^{-3}T$

505.12-2000 K: $\Delta Hr^\circ = 17.444 - 1.551\times10^{-3}T - 0.478\times10^{-6}T^{2} + 195.000T^{-1}$

$\Delta Gr^\circ = 17.444 + 1.551\times10^{-3}T\ln T + 0.478\times10^{-6}T^{2} + 97.500T^{-1} - 26.177\times10^{-3}T$

Source: Data from Mills (332).

$SrAl_2O_4(c)$
Strontium Aluminate
[Formation: $Sr(c,l,g) + 2Al(c,l) + 2O_2(g) = SrAl_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	28.449	30.800	30.800	0	-560.930	-533.124	390.785
300	28.626	30.977	30.807	.051	-560.939	-532.953	388.251
400	34.903	40.198	32.018	3.272	-560.993	-523.603	286.079
500	37.872	48.341	34.489	6.926	-560.748	-514.279	224.788
600	39.539	55.406	37.399	10.804	-560.424	-505.013	183.949
700	40.590	61.585	40.422	14.814	-560.125	-495.802	154.794
800	41.314	67.056	43.417	18.911	-559.910	-486.633	132.940
828	41.464	68.480	44.241	20.070	-559.870	-484.069	127.768
828	41.464	68.480	44.241	20.070	-560.050	-484.069	127.768
900	41.848	71.954	46.320	23.071	-559.975	-477.465	115.943
932	41.991	73.420	47.226	24.413	-559.952	-474.532	111.274
932	41.444	73.911	47.226	24.871	-559.494	-474.532	111.274
933.61	41.455	73.983	47.271	24.938	-559.494	-474.385	111.048
933.61	41.455	73.983	47.271	24.938	-564.654	-474.385	111.048
1000	41.920	76.846	49.141	27.705	-564.595	-467.968	102.273
1041	42.207	78.536	50.266	29.430	-564.547	-464.007	97.413
1041	42.207	78.536	50.266	29.430	-566.507	-464.007	97.413
1100	42.620	80.874	51.845	31.932	-566.388	-458.201	91.035
1200	43.320	84.612	54.421	36.229	-566.145	-448.373	81.659
1300	44.020	88.107	56.879	40.596	-565.848	-438.573	73.730
1400	44.720	91.395	59.229	45.033	-565.497	-428.794	66.937
1500	45.420	94.504	61.477	49.540	-565.088	-419.047	61.054
1600	46.120	97.458	63.635	54.117	-564.623	-409.324	55.910
1654.1	46.499	98.998	64.766	56.622	-564.346	-404.078	53.389
1654.1	46.499	98.998	64.766	56.622	-597.076	-404.078	53.389
1700	46.820	100.275	65.708	58.764	-596.672	-398.729	51.259
1800	47.520	102.971	67.704	63.481	-595.747	-387.109	47.001
1900	48.220	105.559	69.628	68.268	-594.766	-375.542	43.197
2000	48.920	108.050	71.488	73.125	-593.727	-364.033	39.779

Phase changes:
828 K, α - β transition point of Sr; ΔH° = 0.180 kcal/mol.
932 K, α - β transition point of $SrAl_2O_4$; ΔH° = 0.458 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-932 K: $C_p^\circ = 42.271 + 1.282\times10^{-3}T - 12.627\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 42.271\times10^{-3}T + 0.641\times10^{-6}T^2 + 12.627\times10^{2}T^{-1} - 16.895$
932-2500 K: $C_p^\circ = 34.910 + 7.004\times10^{-3}T + 0.053\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 34.910\times10^{-3}T + 3.502\times10^{-6}T^2 - 0.053\times10^{2}T^{-1} - 10.701$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf^\circ = -568.684 + 14.033\times10^{-3}T - 6.351\times10^{-6}T^2 + 1232.800T^{-1}$
$\Delta Gf^\circ = -568.684 - 14.033\times10^{-3}T\ln T + 6.351\times10^{-6}T^2 + 616.400T^{-1} + 190.396\times10^{-3}T$
828-932 K: $\Delta Hf^\circ = -566.921 + 9.627\times10^{-3}T - 3.819\times10^{-6}T^2 + 1207.100T^{-1}$
$\Delta Gf^\circ = -566.921 - 9.627\times10^{-3}T\ln T + 3.819\times10^{-6}T^2 + 603.550T^{-1} + 160.778\times10^{-3}T$
932-933.61 K: $\Delta Hf^\circ = -560.727 + 2.266\times10^{-3}T - 0.958\times10^{-6}T^2 - 60.900T^{-1}$
$\Delta Gf^\circ = -560.727 - 2.266\times10^{-3}T\ln T + 0.958\times10^{-6}T^2 - 30.450T^{-1} + 107.199\times10^{-3}T$
933.61-1041 K: $\Delta Hf^\circ = -563.262 - 3.730\times10^{-3}T + 2.496\times10^{-6}T^2 - 95.700T^{-1}$
$\Delta Gf^\circ = -563.262 + 3.730\times10^{-3}T\ln T - 2.496\times10^{-6}T^2 - 47.850T^{-1} + 72.152\times10^{-3}T$
1041-1654.1 K: $\Delta Hf^\circ = -565.847 - 3.130\times10^{-3}T + 2.496\times10^{-6}T^2 - 95.700T^{-1}$
$\Delta Gf^\circ = -565.847 + 3.130\times10^{-3}T\ln T - 2.496\times10^{-6}T^2 - 47.850T^{-1} + 78.804\times10^{-3}T$
1654.1-2000 K: $\Delta Hf^\circ = -594.724 - 5.003\times10^{-3}T + 3.471\times10^{-6}T^2 - 5756.400T^{-1}$
$\Delta Gf^\circ = -594.724 + 5.003\times10^{-3}T\ln T - 3.471\times10^{-6}T^2 - 2878.200T^{-1} + 85.028\times10^{-3}T$

Source: Data from Fegley (144).

$SrC_2(c)$
Strontium Dicarbide
[Formation: $Sr(c,l) + 2C(c) = SrC_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.068	17.000	17.000	0	-18.000	-18.524	13.578
300	15.099	17.093	17.000	.028	-17.992	-18.527	13.497
400	16.293	21.620	17.610	1.604	-17.563	-18.771	10.256
500	16.990	25.335	18.793	3.271	-17.229	-19.113	8.354
600	17.492	28.479	20.152	4.996	-17.000	-19.513	7.107
700	17.902	31.207	21.541	6.766	-16.869	-19.945	6.227
800	18.263	33.622	22.903	8.575	-16.826	-20.388	5.570
828	18.356	34.252	23.276	9.088	-16.830	-20.512	5.414
828	18.356	34.252	23.276	9.088	-17.010	-20.512	5.414
900	18.595	35.792	24.216	10.418	-17.034	-20.818	5.055
1000	18.910	37.768	25.475	12.293	-17.073	-21.236	4.641

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase change: 828 K, α - β transition point of Sr; ΔH° = 0.180 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 16.400 + 2.700\times10^{-3}T - 1.900\times10^{5}T^{-2}$

$H° - H°_{298} = 16.400\times10^{-3}T + 1.350\times10^{-6}T^{2} + 1.900\times10^{2}T^{-1} - 5.647$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf° = -18.749 + 4.770\times10^{-3}T - 2.714\times10^{-6}T^{2} - 128.900T^{-1}$

$\Delta Gf° = -18.749 - 4.770\times10^{-3}T\ln T + 2.714\times10^{-6}T^{2} - 64.450T^{-1} + 27.848\times10^{-3}T$

828-1000 K: $\Delta Hf° = -16.985 + 0.364\times10^{-3}T - 0.182\times10^{-6}T^{2} - 154.600T^{-1}$

$\Delta Gf° = -16.985 - 0.364\times10^{-3}T\ln T + 0.182\times10^{-6}T^{2} - 77.300T^{-1} - 1.770\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Entropy at 298 K from Flowers (153). Other data are those estimated by Barin (23).

$SrCO_3(c)$
Strontium Carbonate
[Formation: $Sr(c,l) + C(c) + 1.5O_2(g) = SrCO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	19.460	23.200	23.200	0	-291.284	-272.149	199.488
300	19.530	23.320	23.200	.036	-291.283	-272.030	198.171
400	23.440	29.620	24.033	2.235	-291.053	-265.640	145.137
500	24.550	34.990	25.708	4.641	-290.759	-259.324	113.349
600	25.290	39.530	27.642	7.133	-290.518	-253.059	92.175
700	26.140	43.490	29.629	9.703	-290.331	-246.832	77.063
800	27.180	47.040	31.581	12.367	-290.171	-240.626	65.735
828	27.524	47.981	32.120	13.133	-290.127	-238.893	63.055
828	27.524	47.981	32.120	13.133	-290.307	-238.893	63.055
900	28.410	50.310	33.481	15.146	-290.177	-234.426	56.926
1000	29.810	53.380	35.325	18.055	-289.915	-228.250	49.883
1041	30.441	54.591	36.060	19.290	-289.776	-225.724	47.388
1041	30.441	54.591	36.060	19.290	-291.736	-225.724	47.388
1100	31.350	56.290	37.097	21.112	-291.465	-221.976	44.102
1197	32.950	59.110	38.800	24.312	-290.835	-215.926	39.424
1197	34.600	62.870	38.800	28.810	-286.337	-215.926	39.424
1200	34.600	62.960	38.865	28.914	-286.313	-215.755	39.294
1300	34.600	65.730	40.823	32.379	-285.522	-209.904	35.288
1400	34.600	68.300	42.698	35.843	-284.753	-204.120	31.864
1500	34.600	70.690	44.484	39.309	-284.000	-198.386	28.904

Phase changes: 828 K, α − β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1197 K, α − β transition point of $SrCO_3$; ΔH° = 4.498 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1197 K: $Cp° = 22.556 + 7.816\times10^{-3}T - 4.824\times10^{5}T^{-2}$
$H°-H°_{298} = 22.556\times10^{-3}T + 3.908\times10^{-6}T^2 + 4.824\times10^{2}T^{-1} - 8.690$
1197-1500 K: $Cp° = 34.600$
$H°-H°_{298} = 34.600\times10^{-3}T - 12.606$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf° = -293.243 + 3.599\times10^{-3}T - 0.145\times10^{-6}T^2 + 268.000T^{-1}$
$\Delta Gf° = -293.243 - 3.599\times10^{-3}T\ln T + 0.145\times10^{-6}T^2 + 134.000T^{-1} + 89.705\times10^{-3}T$
828-1041 K: $\Delta Hf° = -291.480 - 0.807\times10^{-3}T + 2.388\times10^{-6}T^2 + 242.300T^{-1}$
$\Delta Gf° = -291.480 + 0.807\times10^{-3}T\ln T - 2.388\times10^{-6}T^2 + 121.150T^{-1} + 60.087\times10^{-3}T$
1041-1197 K: $\Delta Hf° = -294.064 - 0.207\times10^{-3}T + 2.388\times10^{-6}T^2 + 242.300T^{-1}$
$\Delta Gf° = -294.064 + 0.207\times10^{-3}T\ln T - 2.388\times10^{-6}T^2 + 121.150T^{-1} + 66.739\times10^{-3}T$
1197-1500 K: $\Delta Hf° = -297.981 + 11.837\times10^{-3}T - 1.521\times10^{-6}T^2 - 240.100T^{-1}$
$\Delta Gf° = -297.981 - 11.837\times10^{-3}T\ln T + 1.521\times10^{-6}T^2 - 120.050T^{-1} + 150.863\times10^{-3}T$

Source: Data from Chang (74).

$SrH(g)$
Strontium Monohydride (ideal gas)
[Formation: $Sr(c,l,g) + 0.5H_2(g) = SrH(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.201	50.822	50.822	0	52.400	45.626	-33.445
300	7.207	50.866	50.823	.013	52.395	45.584	-33.208
400	7.531	52.983	51.108	.750	52.125	43.355	-23.688
500	7.846	54.698	51.660	1.519	51.846	41.195	-18.006
600	8.107	56.153	52.291	2.317	51.552	39.091	-14.239
700	8.313	57.419	52.935	3.139	51.232	37.039	-11.564
800	8.476	58.540	53.568	3.978	50.870	35.034	-9.571
828	8.513	58.832	53.741	4.216	50.760	34.482	-9.101
828	8.513	58.832	53.741	4.216	50.580	34.482	-9.101
900	8.607	59.546	54.176	4.833	50.293	33.095	-8.037
1000	8.714	60.458	54.759	5.699	49.900	31.207	-6.820
1041	8.751	60.809	54.990	6.057	49.740	30.444	-6.391
1041	8.751	60.809	54.990	6.057	47.780	30.444	-6.391
1100	8.805	61.293	55.316	6.575	47.589	29.466	-5.854
1200	8.885	62.063	55.846	7.460	47.265	27.833	-5.069
1300	8.956	62.777	56.352	8.352	46.945	26.226	-4.409
1400	9.021	63.443	56.835	9.251	46.626	24.646	-3.847
1500	9.082	64.068	57.297	10.156	46.307	23.085	-3.363
1600	9.140	64.656	57.739	11.067	45.990	21.548	-2.943
1654.1	9.169	64.960	57.969	11.563	45.818	20.726	-2.738
1654.1	9.169	64.960	57.969	11.563	13.088	20.726	-2.738
1700	9.194	65.211	58.162	11.984	13.099	20.936	-2.691
1800	9.244	65.738	58.568	12.906	13.124	21.396	-2.598
1900	9.291	66.239	58.958	13.833	13.148	21.857	-2.514
2000	9.333	66.717	59.335	14.764	13.170	22.313	-2.438

Phase changes: 828 K, α − β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.815 + 0.872\times10^{-3}T - 0.776\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 7.815\times10^{-3}T + 0.436\times10^{-6}T^{2} + 0.776\times10^{2}T^{-1} - 2.629$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf^\circ = 52.233 - 0.007\times10^{-3}T - 2.306\times10^{-6}T^{2} + 111.550T^{-1}$
$\Delta Gf^\circ = 52.233 + 0.007\times10^{-3}T\ln T + 2.306\times10^{-6}T^{2} + 55.775T^{-1} - 23.513\times10^{-3}T$
828-1041 K: $\Delta Hf^\circ = 53.996 - 4.413\times10^{-3}T + 0.226\times10^{-6}T^{2} + 85.850T^{-1}$
$\Delta Gf^\circ = 53.996 + 4.413\times10^{-3}T\ln T - 0.226\times10^{-6}T^{2} + 42.925T^{-1} - 53.131\times10^{-3}T$
1041-1654.1 K: $\Delta Hf^\circ = 51.412 - 3.813\times10^{-3}T + 0.226\times10^{-6}T^{2} + 85.850T^{-1}$
$\Delta Gf^\circ = 51.412 + 3.813\times10^{-3}T\ln T - 0.226\times10^{-6}T^{2} + 42.925T^{-1} - 46.479\times10^{-3}T$
1654.1-2000 K: $\Delta Hf^\circ = 22.534 - 5.686\times10^{-3}T + 1.201\times10^{-6}T^{2} - 5574.850T^{-1}$
$\Delta Gf^\circ = 22.534 + 5.686\times10^{-3}T\ln T - 1.201\times10^{-6}T^{2} - 2787.425T^{-1} - 40.255\times10^{-3}T$

Source: Data from Gurvich (196).

$SrH_2(c,l)$
Strontium Dihydride
[Formation: $Sr(c,l,g) + H_2(g) = SrH_2(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	10.516	12.428	12.428	0	-43.000	-33.674	24.684
300	10.531	12.493	12.430	.019	-43.006	-33.617	24.490
400	11.308	15.629	12.851	1.111	-43.267	-30.446	16.635
500	12.086	18.236	13.674	2.281	-43.495	-27.214	11.895
600	12.863	20.508	14.628	3.528	-43.690	-23.940	8.720
700	13.641	22.550	15.616	4.854	-43.857	-20.635	6.442
800	14.418	24.422	16.601	6.257	-44.008	-17.306	4.728
828	14.636	24.922	16.874	6.664	-44.049	-16.371	4.321
828	14.636	24.922	16.874	6.664	-44.229	-16.371	4.321
900	15.196	26.165	17.568	7.737	-44.316	-13.946	3.386
1000	15.973	27.806	18.510	9.296	-44.375	-10.566	2.309
1041	16.292	28.454	18.889	9.957	-44.379	-9.179	1.927
1041	16.292	28.454	18.889	9.957	-46.339	-9.179	1.927
1100	16.751	29.365	19.427	10.932	-46.289	-7.075	1.406
1128	16.968	29.789	19.678	11.405	-46.256	-6.077	1.177
1128	16.970	31.314	19.678	13.125	-44.536	-6.077	1.177
1200	16.970	32.364	20.408	14.347	-44.450	-3.624	.660
1300	16.970	33.723	21.381	16.044	-44.339	-.227	.038
1323	16.970	34.020	21.598	16.434	-44.315	.553	-.091
1323	17.925	38.175	21.598	21.931	-38.818	.553	-.091
1400	17.925	39.189	22.538	23.311	-38.668	2.841	-.443
1500	17.925	40.426	23.690	25.104	-38.482	5.798	-.845
1600	17.925	41.583	24.773	26.896	-38.307	8.744	-1.194
1654.1	17.925	42.179	25.333	27.866	-38.216	10.334	-1.365
1654.1	17.925	42.179	25.333	27.866	-70.946	10.334	-1.365
1700	17.925	42.670	25.794	28.689	-70.715	12.585	-1.618
1800	17.925	43.694	26.760	30.481	-70.218	17.471	-2.121
1900	17.925	44.664	27.678	32.274	-69.731	22.330	-2.568
2000	17.925	45.583	28.550	34.066	-69.256	27.162	-2.968

Phase changes:
828 K, α - β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1128 K, α - β transition point of SrH_2; ΔH° = 1.720 kcal/mol.
1363 K, melting point of SrH_2; ΔH° = 5.497 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1128 K: $Cp° = 8.182 + 7.796\times10^{-3}T + 0.009\times10^{5}T^{-2}$
$H°-H°_{298} = 8.182\times10^{-3}T + 3.898\times10^{-6}T^{2} - 0.009\times10^{2}T^{-1} - 2.783$
1128-1323 K: $Cp° = 16.969$
$H°-H°_{298} = 16.969\times10^{-3}T - 6.016$
1323-2000 K: $Cp° = 17.925$
$H°-H°_{298} = 17.925\times10^{-3}T - 1.784$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf° = -42.368 - 2.868\times10^{-3}T + 0.947\times10^{-6}T^{2} + 41.300T^{-1}$
$\Delta Gf° = -42.368 + 2.868\times10^{-3}T\ln T - 0.947\times10^{-6}T^{2} + 20.650T^{-1} + 12.867\times10^{-3}T$
828-1041 K: $\Delta Hf° = -40.604 - 7.274\times10^{-3}T + 3.479\times10^{-6}T^{2} + 15.600T^{-1}$
$\Delta Gf° = -40.604 + 7.274\times10^{-3}T\ln T - 3.479\times10^{-6}T^{2} + 7.800T^{-1} - 16.751\times10^{-3}T$
1041-1128 K: $\Delta Hf° = -43.189 - 6.674\times10^{-3}T + 3.479\times10^{-6}T^{2} + 15.600T^{-1}$
$\Delta Gf° = -43.189 + 6.674\times10^{-3}T\ln T - 3.479\times10^{-6}T^{2} + 7.800T^{-1} - 10.099\times10^{-3}T$
1128-1323 K: $\Delta Hf° = -46.422 + 2.113\times10^{-3}T - 0.419\times10^{-6}T^{2} + 16.500T^{-1}$
$\Delta Gf° = -46.422 - 2.113\times10^{-3}T\ln T + 0.419\times10^{-6}T^{2} + 8.250T^{-1} + 50.126\times10^{-3}T$
1323-1654.1 K: $\Delta Hf° = -42.189 + 3.069\times10^{-3}T - 0.419\times10^{-6}T^{2} + 16.500T^{-1}$
$\Delta Gf° = -42.189 - 3.069\times10^{-3}T\ln T + 0.419\times10^{-6}T^{2} + 8.250T^{-1} + 53.798\times10^{-3}T$
1654.1-2000 K: $\Delta Hf° = -71.067 + 1.196\times10^{-3}T + 0.556\times10^{-6}T^{2} - 5644.200T^{-1}$
$\Delta Gf° = -71.067 - 1.196\times10^{-3}T\ln T - 0.556\times10^{-6}T^{2} - 2822.100T^{-1} + 60.023\times10^{-3}T$

Source: Data from Gurvich (196).

$Sr(IO_3)_2(c)$
Strontium Iodate
[Formation: $Sr(c) + I_2(c,l,g) + 3O_2(g) = Sr(IO_3)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	44.200	56.000	56.000	0	-243.600	-204.461	149.872
300	44.300	56.270	56.003	.080	-243.595	-204.218	148.771
350	47.810	63.380	56.551	2.390	-243.332	-197.672	123.431
386.8	49.966	68.270	57.450	4.185	-243.113	-192.887	108.984
386.8	49.966	68.270	57.450	4.185	-246.822	-192.887	108.984
400	50.740	69.960	57.835	4.850	-246.786	-191.048	104.382
450	53.330	76.090	59.512	7.460	-246.570	-184.082	89.401
458.4	53.730	77.080	59.825	7.910	-246.526	-182.916	87.207
458.4	53.730	77.080	59.825	7.910	-256.547	-182.916	87.207
500	55.710	81.830	61.470	10.180	-255.866	-176.267	77.045
550	57.940	87.240	63.567	13.020	-254.963	-168.350	66.895
600	60.090	92.380	65.747	15.980	-253.970	-160.513	58.466
650	62.160	97.270	67.993	19.030	-252.917	-152.773	51.366
700	64.190	101.950	70.250	22.190	-251.784	-145.110	45.305
750	66.180	106.450	72.517	25.450	-250.581	-137.536	40.077

Phase chnages: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-750 K: $Cp° = 39.550 + 36.854 \times 10^{-3}T - 5.677 \times 10^{5}T^{-2}$
$H° - H°_{298} = 39.550 \times 10^{-3}T + 18.427 \times 10^{-6}T^{2} + 5.677 \times 10^{2}T^{-1} - 15.334$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -246.398 + 0.389 \times 10^{-3}T + 12.894 \times 10^{-6}T^{2} + 457.800T^{-1}$
$\Delta Gf° = -246.398 - 0.389 \times 10^{-3}T\ln T - 12.894 \times 10^{-6}T^{2} + 228.900T^{-1} + 144.142 \times 10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -247.853 - 6.015 \times 10^{-3}T + 14.386 \times 10^{-6}T^{2} + 457.800T^{-1}$
$\Delta Gf° = -247.853 + 6.015 \times 10^{-3}T\ln T - 14.386 \times 10^{-6}T^{2} + 228.900T^{-1} + 110.327 \times 10^{-3}T$
458.4-750 K: $\Delta Hf° = -262.566 + 4.325 \times 10^{-3}T + 14.318 \times 10^{-6}T^{2} + 442.500T^{-1}$
$\Delta Gf° = -262.566 - 4.325 \times 10^{-3}T\ln T - 14.318 \times 10^{-6}T^{2} + 221.250T^{-1} + 205.790 \times 10^{-3}T$

Source: Enthalpy of formation and entropy at 298 K from Parker (391). Other data based on David (109).

$Sr_3N_2(c)$
Tristrontium Dinitride
[Formation: $3Sr(c,l) + N_2(g) = Sr_3N_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	30.988	32.200	32.200	0	-93.500	-78.273	57.375
300	31.000	32.392	32.200	.058	-93.491	-78.179	56.952
400	31.650	41.399	33.424	3.190	-93.033	-73.145	39.964
500	32.300	48.531	35.755	6.388	-92.635	-68.220	29.818
600	32.950	54.478	38.395	9.650	-92.312	-63.370	23.082
700	33.600	59.606	41.066	12.978	-92.084	-58.566	18.285
800	34.250	64.135	43.673	16.370	-91.979	-53.788	14.694
828	34.432	65.316	44.385	17.332	-91.975	-52.451	13.844
828	34.432	65.316	44.385	17.332	-92.515	-52.451	13.844
900	34.900	68.206	46.175	19.828	-92.511	-48.965	11.890
1000	35.550	71.917	48.567	23.350	-92.464	-44.128	9.644
1041	35.817	73.351	49.515	24.813	-92.430	-42.145	8.848
1041	35.817	73.351	49.515	24.813	-98.310	-42.145	8.848
1100	36.200	75.336	50.847	26.938	-98.136	-38.968	7.742
1200	36.850	78.514	53.022	30.590	-97.804	-33.604	6.120
1300	37.500	81.489	55.098	34.308	-97.417	-28.269	4.752

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 828 K, α − β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 29.050 + 6.500\times10^{-3}T$
$H^\circ - H^\circ_{298} = 29.050\times10^{-3}T + 3.250\times10^{-6}T^2 - 8.950$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf^\circ = -95.956 + 8.751\times10^{-3}T - 4.935\times10^{-6}T^2 + 85.000T^{-1}$
$\Delta Gf^\circ = -95.956 - 8.751\times10^{-3}T\ln T + 4.935\times10^{-6}T^2 + 42.500T^{-1} + 107.216\times10^{-3}T$
828-1041 K: $\Delta Hf^\circ = -90.666 - 4.467\times10^{-3}T + 2.661\times10^{-6}T^2 + 7.900T^{-1}$
$\Delta Gf^\circ = -90.666 + 4.467\times10^{-3}T\ln T - 2.661\times10^{-6}T^2 + 3.950T^{-1} + 18.361\times10^{-3}T$
1041-1300 K: $\Delta Hf^\circ = -98.419 - 2.667\times10^{-3}T + 2.661\times10^{-6}T^2 + 7.900T^{-1}$
$\Delta Gf^\circ = -98.419 + 2.667\times10^{-3}T\ln T - 2.661\times10^{-6}T^2 + 3.950T^{-1} + 38.316\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Other data are those estimated by Barin (23).

$Sr(NO_3)_2(c)$
Strontium Nitrate
[Formation: $Sr(c) + N_2(g) + 3O_2(g) = Sr(NO_3)_2(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	35.900	46.500	46.500	0	-233.800	-186.458	136.676
300	36.010	46.720	46.500	.070	-233.794	-186.160	135.616
400	41.630	57.870	47.970	3.960	-233.390	-170.329	93.062
500	46.720	67.720	50.960	8.380	-232.565	-154.654	67.599
600	51.300	76.650	54.517	13.280	-231.385	-139.184	50.697
700	55.350	84.870	58.270	18.620	-229.897	-123.927	38.691
800	58.860	92.490	62.077	24.330	-228.172	-108.908	29.752
828	59.689	94.529	63.141	25.990	-227.651	-104.743	27.646
828	59.689	94.529	63.141	25.990	-227.831	-104.743	27.646
900	61.820	99.600	65.856	30.370	-226.410	-94.096	22.849

Phase change: 828 K, α − β transition point of Sr; ΔH° = 0.180 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-900 K:

$$Cp° = 29.330 + 37.886\times10^{-3}T - 4.201\times10^{5}T^{-2}$$

$$H°-H°_{298} = 29.330\times10^{-3}T + 18.943\times10^{-6}T^{2} + 4.201\times10^{2}T^{-1} - 11.838$$

Formation equations (kcal/mol):

298.15-828 K:

$$\Delta Hf° = -235.104 - 3.471\times10^{-3}T + 14.313\times10^{-6}T^{2} + 318.100T^{-1}$$

$$\Delta Gf° = -235.104 + 3.471\times10^{-3}T\ln T - 14.313\times10^{-6}T^{2} + 159.050T^{-1} + 145.862\times10^{-3}T$$

828-900 K:

$$\Delta Hf° = -233.341 - 7.877\times10^{-3}T + 16.845\times10^{-6}T^{2} + 292.400T^{-1}$$

$$\Delta Gf° = -233.341 + 7.877\times10^{-3}T\ln T - 16.845\times10^{-6}T^{2} + 146.200T^{-1} + 116.243\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Taylor (490). High-temperature data based on Taylor (490).

SrOH(g)

Strontium Monohydroxide (ideal gas)

[Formation: $Sr(c,l,g) + 0.5H_2(g) + 0.5O_2(g) = SrOH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	10.984	58.891	58.891	0	-49.120	-50.994	37.379
300	11.003	58.959	58.892	.020	-49.125	-51.006	37.157
400	11.732	62.235	59.333	1.161	-49.345	-51.598	28.191
500	12.128	64.900	60.188	2.356	-49.564	-52.136	22.788
600	12.374	67.134	61.164	3.582	-49.807	-52.628	19.170
700	12.556	69.056	62.157	4.829	-50.091	-53.077	16.571
800	12.711	70.743	63.128	6.092	-50.429	-53.482	14.611
828	12.751	71.181	63.393	6.448	-50.533	-53.588	14.144
828	12.751	71.181	63.393	6.448	-50.713	-53.588	14.144
900	12.855	72.248	64.059	7.370	-50.990	-53.825	13.070
1000	12.995	73.610	64.947	8.663	-51.370	-54.120	11.828
1041	13.050	74.133	65.299	9.197	-51.524	-54.229	11.385
1041	13.050	74.133	65.299	9.197	-53.484	-54.229	11.385
1100	13.130	74.855	65.792	9.969	-53.670	-54.266	10.782
1200	13.259	76.003	66.595	11.289	-53.982	-54.305	9.890
1300	13.382	77.069	67.361	12.621	-54.291	-54.320	9.132
1400	13.496	78.065	68.090	13.965	-54.597	-54.311	8.478
1500	13.603	79.000	68.787	15.320	-54.901	-54.281	7.909
1600	13.702	79.881	69.453	16.685	-55.203	-54.229	7.407
1654.1	13.751	80.337	69.801	17.428	-55.365	-54.192	7.160
1654.1	13.751	80.337	69.801	17.428	-88.095	-54.192	7.160
1700	13.793	80.714	70.090	18.060	-88.076	-53.253	6.846
1800	13.877	81.505	70.703	19.444	-88.033	-51.205	6.217
1900	13.955	82.258	71.292	20.835	-87.992	-49.161	5.655
2000	14.028	82.975	71.858	22.234	-87.951	-47.118	5.149

*Data except enthalpy of formation at 298 K estimated.

Phase changes:
828 K, α - β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:
$Cp° = 12.103 + 1.026x10^{-3}T - 1.267x10^{5}T^{-2}$
$H°- H°_{298} = 12.103x10^{-3}T + 0.513x10^{-6}T^{2} + 1.267x10^{2}T^{-1} - 4.079$

Formation equations (kcal/mol):

298.15-828 K:
$ΔHf° = -49.561 + 0.666x10^{-3}T - 2.480x10^{-6}T^{2} + 138.050T^{-1}$
$ΔGf° = -49.561 - 0.666x10^{-3}TlnT + 2.480x10^{-6}T^{2} + 69.025T^{-1} - 2.527x10^{-3}T$

828-1041 K:
$ΔHf° = -47.798 - 3.740x10^{-3}T + 0.052x10^{-6}T^{2} + 112.350T^{-1}$
$ΔGf° = -47.798 + 3.740x10^{-3}TlnT - 0.052x10^{-6}T^{2} + 56.175T^{-1} - 32.145x10^{-3}T$

1041-1654.1 K:
$ΔHf° = -50.382 - 3.140x10^{-3}T + 0.052x10^{-6}T^{2} + 112.350T^{-1}$
$ΔGf° = -50.382 + 3.140x10^{-3}TlnT - 0.052x10^{-6}T^{2} + 56.175T^{-1} - 25.494x10^{-3}T$

1654.1-2000 K:
$ΔHf° = -79.260 - 5.013x10^{-3}T + 1.027x10^{-6}T^{2} - 5548.350T^{-1}$
$ΔGf° = -79.260 + 5.013x10^{-3}TlnT - 1.027x10^{-6}T^{2} - 2774.175T^{-1} - 19.269x10^{-3}T$

Source: Data from Chase (82) who estimated molecular constants.

$Sr(OH)_2(c,l)$
Strontium Dihydroxide
[Formation: $Sr(c,l) + H_2(g) + O_2(g) = Sr(OH)_2(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	17.900	23.200	23.200	0	-231.570	-210.845	154.552
300	17.960	23.311	23.201	.033	-231.575	-210.717	153.505
400	21.140	28.913	23.943	1.988	-231.683	-203.740	111.317
500	24.320	33.972	25.450	4.261	-231.539	-196.765	86.005
600	27.490	38.685	27.267	6.851	-231.146	-189.844	69.150
700	30.670	43.162	29.221	9.759	-230.509	-183.008	57.137
783	33.310	46.742	30.886	12.415	-229.799	-177.413	49.519
783	37.700	53.158	30.886	17.439	-224.775	-177.413	49.519
800	37.700	53.968	31.368	18.080	-224.540	-176.387	48.186
828	37.700	55.265	32.154	19.136	-224.158	-174.709	46.114
828	37.700	55.265	32.154	19.136	-224.338	-174.709	46.114
900	37.700	58.408	34.130	21.850	-223.372	-170.433	41.386
1000	37.700	62.380	36.760	25.620	-222.047	-164.622	35.978
1041	37.700	63.895	37.799	27.166	-221.510	-162.278	34.069
1041	37.700	63.895	37.799	27.166	-223.470	-162.278	34.069
1100	37.700	65.973	39.255	29.390	-222.666	-158.832	31.557

*Entropy at 298 K estimated.

Phase changes: 783 K, melting point of $Sr(OH)_2$; ΔH° = 5.024 kcal/mol.
828 K, α – β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-783 K: $Cp° = 8.425 + 31.784\times10^{-3}T - 0.001\times10^{5}T^{-2}$
$H°-H°_{298} = 8.425\times10^{-3}T + 15.892\times10^{-6}T^{2} + 0.001\times10^{2}T^{-1} - 3.925$
783-1100 K: $Cp° = 37.700$
$H°-H°_{298} = 37.700\times10^{-3}T - 12.080$

Formation equations (kcal/mol):

298.15-783 K: $\Delta Hf° = -229.728 - 9.855\times10^{-3}T + 12.438\times10^{-6}T^{2} - 2.900T^{-1}$
$\Delta Gf° = -229.728 + 9.855\times10^{-3}T\ln T - 12.438\times10^{-6}T^{2} - 1.450T^{-1} + 10.908\times10^{-3}T$
783-828 K: $\Delta Hf° = -237.883 + 19.420\times10^{-3}T - 3.454\times10^{-6}T^{2} - 3.000T^{-1}$
$\Delta Gf° = -237.883 - 19.420\times10^{-3}T\ln T + 3.454\times10^{-6}T^{2} - 1.500T^{-1} + 203.943\times10^{-3}T$
828-1041 K: $\Delta Hf° = -236.119 + 15.014\times10^{-3}T - 0.922\times10^{-6}T^{2} - 28.700T^{-1}$
$\Delta Gf° = -236.119 - 15.014\times10^{-3}T\ln T + 0.922\times10^{-6}T^{2} - 14.350T^{-1} + 174.324\times10^{-3}T$
1041-1100 K: $\Delta Hf° = -238.704 + 15.614\times10^{-3}T - 0.922\times10^{-6}T^{2} - 28.700T^{-1}$
$\Delta Gf° = -238.704 - 15.614\times10^{-3}T\ln T + 0.922\times10^{-6}T^{2} - 14.350T^{-1} + 180.976\times10^{-3}T$

Source: Data from Chase (82) who estimated entropy at 298 K.

$Sr(OH)_2(g)$
Strontium Dihydroxide (ideal gas)
[Formation: $Sr(c,l,g) + H_2(g) + O_2(g) = Sr(OH)_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	18.214	72.880	72.880	0	-142.400	-136.487	100.046
300	18.250	72.993	72.880	.034	-142.404	-136.450	99.403
400	19.645	78.457	73.617	1.936	-142.565	-134.439	73.453
500	20.392	82.928	75.044	3.942	-142.688	-132.392	57.868
600	20.856	86.690	76.682	6.005	-142.822	-130.323	47.469
700	21.199	89.931	78.347	8.109	-142.989	-128.226	40.033
800	21.495	92.782	79.977	10.244	-143.206	-126.104	34.450
828	21.573	93.523	80.423	10.847	-143.277	-125.505	33.126
828	21.573	93.523	80.423	10.847	-143.457	-125.505	33.126
900	21.775	95.330	81.544	12.407	-143.645	-123.936	30.095
1000	22.047	97.638	83.039	14.599	-143.898	-121.731	26.604
1041	22.156	98.526	83.632	15.505	-144.000	-120.820	25.365
1041	22.156	98.526	83.632	15.505	-145.960	-120.820	25.365
1100	22.312	99.752	84.464	16.817	-146.069	-119.392	23.721
1200	22.567	101.704	85.820	19.061	-146.249	-116.957	21.301
1300	22.808	103.520	87.113	21.329	-146.423	-114.511	19.251
1400	23.035	105.219	88.346	23.622	-146.590	-112.049	17.491
1500	23.245	106.815	89.524	25.936	-146.753	-109.577	15.965
1600	23.439	108.322	90.653	28.270	-146.913	-107.094	14.628
1654.1	23.535	109.103	91.244	29.541	-146.998	-105.744	13.971
1654.1	23.535	109.103	91.244	29.541	-179.728	-105.744	13.971
1700	23.617	109.748	91.734	30.623	-179.643	-103.694	13.331
1800	23.780	111.103	92.774	32.993	-179.456	-99.232	12.048
1900	23.929	112.393	93.772	35.379	-179.270	-94.779	10.902
2000	24.064	113.624	94.735	37.779	-179.086	-90.338	9.872

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 828 K, α − β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 20.337 + 1.980\times10^{-3}T - 2.412\times10^{5}T^{-2}$
$H°-H°_{298} = 20.337\times10^{-3}T + 0.990\times10^{-6}T^{2} + 2.412\times10^{2}T^{-1} - 6.960$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf° = -143.593 + 2.057\times10^{-3}T - 2.464\times10^{-6}T^{2} + 238.200T^{-1}$
$\Delta Gf° = -143.593 - 2.057\times10^{-3}T\ln T + 2.464\times10^{-6}T^{2} + 119.100T^{-1} + 33.479\times10^{-3}T$
828-1041 K: $\Delta Hf° = -141.830 - 2.349\times10^{-3}T + 0.068\times10^{-6}T^{2} + 212.500T^{-1}$
$\Delta Gf° = -141.830 + 2.349\times10^{-3}T\ln T - 0.068\times10^{-6}T^{2} + 106.250T^{-1} + 3.861\times10^{-3}T$
1041-1654.1 K: $\Delta Hf° = -144.414 - 1.749\times10^{-3}T + 0.068\times10^{-6}T^{2} + 212.500T^{-1}$
$\Delta Gf° = -144.414 + 1.749\times10^{-3}T\ln T - 0.068\times10^{-6}T^{2} + 106.250T^{-1} + 10.513\times10^{-3}T$
1654.1-2000 K: $\Delta Hf° = -173.292 - 3.622\times10^{-3}T + 1.043\times10^{-6}T^{2} - 5448.200T^{-1}$
$\Delta Gf° = -173.292 + 3.622\times10^{-3}T\ln T - 1.043\times10^{-6}T^{2} - 2724.100T^{-1} + 16.737\times10^{-3}T$

Source: Data from Chase (82) who estimated molecular constants.

$SrSiO_3(c)$
Strontium Silicate
[Formation: $Sr(c,l,g) + Si(c,l) + 1.5O_2(g) = SrSiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	20.984	23.100	23.100	0	-390.400	-370.302	271.436
300*	21.069	23.230	23.100	.039	-390.401	-370.177	269.671
400	24.223	29.780	23.973	2.323	-390.349	-363.441	198.572
500	25.904	35.381	25.709	4.836	-390.177	-356.731	155.925
600	27.005	40.207	27.732	7.485	-389.975	-350.062	127.508
700	27.833	44.435	29.822	10.229	-389.779	-343.425	107.221
800	28.515	48.197	31.888	13.047	-389.612	-336.816	92.013
828	28.682	49.181	32.456	13.848	-389.571	-334.968	88.413
828	28.682	49.181	32.456	13.848	-389.751	-334.968	88.413
900	29.112	51.591	33.892	15.929	-389.648	-330.208	80.185
1000	29.656	54.686	35.819	18.867	-389.478	-323.604	70.723
1041	29.865	55.882	36.586	20.087	-389.401	-320.904	67.370
1041	29.865	55.882	36.586	20.087	-391.361	-320.904	67.370
1100	30.166	57.537	37.665	21.859	-391.205	-316.922	62.966
1200	30.652	60.183	39.433	24.900	-390.921	-310.182	56.491
1300	31.122	62.655	41.125	27.989	-390.605	-303.467	51.017
1400	31.580	64.978	42.747	31.124	-390.263	-296.772	46.328
1500	32.029	67.172	44.303	34.304	-389.892	-290.120	42.270
1600	32.472	69.254	45.798	37.529	-389.490	-283.483	38.721
1654.1	32.708	70.337	46.583	39.292	-389.260	-279.879	36.979
1654.1	32.708	70.337	46.583	39.292	-421.990	-279.879	36.979
1687	32.852	70.983	47.052	40.371	-421.734	-277.058	35.892
1687	32.852	70.983	47.052	40.371	-433.816	-277.058	35.892
1700	32.909	71.235	47.236	40.798	-433.705	-275.846	35.462
1800	33.342	73.129	48.623	44.111	-432.832	-266.582	32.367
1900	33.772	74.943	49.960	47.467	-431.927	-257.369	29.604
2000	34.199	76.686	51.253	50.865	-430.990	-248.213	27.123

*Data above 298 K estimated.

Phase changes:
828 K, α − β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:
$Cp° = 26.100 + 4.120\times10^{-3}T - 5.640\times10^{5}T^{-2}$
$H° - H°_{298} = 26.100\times10^{-3}T + 2.060\times10^{-6}T^{2} + 5.640\times10^{2}T^{-1} - 9.857$

Formation equations (kcal/mol):

298.15-828 K:
$\Delta Hf° = -393.165 + 4.982\times10^{-3}T - 1.577\times10^{-6}T^{2} + 423.400T^{-1}$
$\Delta Gf° = -393.165 - 4.982\times10^{-3}T\ln T + 1.577\times10^{-6}T^{2} + 211.700T^{-1} + 102.216\times10^{-3}T$

828-1041 K:
$\Delta Hf° = -391.402 + 0.576\times10^{-3}T + 0.955\times10^{-6}T^{2} + 397.700T^{-1}$
$\Delta Gf° = -391.402 - 0.576\times10^{-3}T\ln T - 0.955\times10^{-6}T^{2} + 198.850T^{-1} + 72.597\times10^{-3}T$

1041-1654.1 K:
$\Delta Hf° = -393.987 + 1.176\times10^{-3}T + 0.955\times10^{-6}T^{2} + 397.700T^{-1}$
$\Delta Gf° = -393.987 - 1.176\times10^{-3}T\ln T - 0.955\times10^{-6}T^{2} + 198.850T^{-1} + 79.249\times10^{-3}T$

1654.1-1687 K:
$\Delta Hf° = -422.864 - 0.697\times10^{-3}T + 1.930\times10^{-6}T^{2} - 5263.000T^{-1}$
$\Delta Gf° = -422.864 + 0.697\times10^{-3}T\ln T - 1.930\times10^{-6}T^{2} - 2631.500T^{-1} + 85.473\times10^{-3}T$

1687-2000 K:
$\Delta Hf° = -435.293 - 1.118\times10^{-3}T + 2.280\times10^{-6}T^{2} - 5164.500T^{-1}$
$\Delta Gf° = -435.293 + 1.118\times10^{-3}T\ln T - 2.280\times10^{-6}T^{2} - 2582.250T^{-1} + 90.287\times10^{-3}T$

Source: Data from Fegley (144) who estimated all above 298 K.

$Sr_2SiO_4(c)$
Distrontium Silicate
[Formation: $2Sr(c,l,g) + Si(c,l) + 2O_2(g) = Sr_2SiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°₂₉₈)/T	H°- H°₂₉₈	ΔHf°	ΔGf°	
298.15	32.082	36.600	36.600	0	-550.800	-523.695	383.874
300*	32.212	36.799	36.602	.059	-550.800	-523.527	381.384
400	36.979	46.805	37.932	3.549	-550.555	-514.466	281.087
500	39.486	55.350	40.584	7.383	-550.127	-505.489	220.946
600	41.102	62.701	43.673	11.417	-549.659	-496.608	180.887
700	42.299	69.131	46.860	15.590	-549.215	-487.802	152.297
800	43.271	74.844	50.007	19.870	-548.832	-479.056	130.870
828	43.507	76.337	50.872	21.085	-548.740	-476.616	125.801
828	43.507	76.337	50.872	21.085	-549.100	-476.616	125.801
900	44.113	79.991	53.058	24.240	-548.864	-470.322	114.208
1000	44.874	84.678	55.988	28.690	-548.496	-461.604	100.882
1041	45.164	86.487	57.154	30.536	-548.334	-458.044	96.162
1041	45.164	86.487	57.154	30.536	-552.254	-458.044	96.162
1100	45.582	88.989	58.795	33.213	-551.936	-452.721	89.946
1200	46.255	92.984	61.480	37.805	-551.364	-443.726	80.813
1300	46.902	96.712	64.048	42.463	-550.748	-434.783	73.093
1400	47.530	100.211	66.508	47.184	-550.092	-425.883	66.482
1500	48.145	103.511	68.866	51.968	-549.391	-417.047	60.763
1600	48.750	106.638	71.130	56.813	-548.648	-408.248	55.763
1654.1	49.072	108.264	72.317	59.459	-548.228	-403.486	53.310
1654.1	49.072	108.264	72.317	59.459	-613.688	-403.486	53.310
1687	49.269	109.232	73.028	61.077	-613.202	-399.314	51.730
1687	49.269	109.232	73.028	61.077	-625.284	-399.314	51.730
1700	49.346	109.611	73.306	61.718	-625.082	-397.569	51.110
1800	49.937	112.448	75.402	66.682	-623.500	-384.226	46.651
1900	50.522	115.164	77.425	71.705	-621.875	-370.976	42.671
2000	51.103	117.770	79.377	76.786	-620.206	-357.822	39.100

*Data above 298 K estimated.

Phase changes:
828 K, α – β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:
$$Cp° = 40.162 + 5.578\times10^{-3}T - 8.660\times10^{5}T^{-2}$$
$$H° - H°_{298} = 40.162\times10^{-3}T + 2.789\times10^{-6}T^{2} + 8.660\times10^{2}T^{-1} - 15.127$$

Formation equations (kcal/mol):

298.15-828 K:
$$\Delta Hf° = -556.151 + 10.835\times10^{-3}T - 3.632\times10^{-6}T^{2} + 728.500T^{-1}$$
$$\Delta Gf° = -556.151 - 10.835\times10^{-3}T\ln T + 3.632\times10^{-6}T^{2} + 364.250T^{-1} + 165.410\times10^{-3}T$$

828-1041 K:
$$\Delta Hf° = -552.624 + 2.023\times10^{-3}T + 1.432\times10^{-6}T^{2} + 677.100T^{-1}$$
$$\Delta Gf° = -552.624 - 2.023\times10^{-3}T\ln T - 1.432\times10^{-6}T^{2} + 338.550T^{-1} + 106.174\times10^{-3}T$$

1041-1654.1 K:
$$\Delta Hf° = -557.794 + 3.223\times10^{-3}T + 1.432\times10^{-6}T^{2} + 677.100T^{-1}$$
$$\Delta Gf° = -557.794 - 3.223\times10^{-3}T\ln T - 1.432\times10^{-6}T^{2} + 338.550T^{-1} + 119.477\times10^{-3}T$$

1654.1-1687 K:
$$\Delta Hf° = -615.548 - 0.523\times10^{-3}T + 3.382\times10^{-6}T^{2} - 10644.301T^{-1}$$
$$\Delta Gf° = -615.548 + 0.523\times10^{-3}T\ln T - 3.382\times10^{-6}T^{2} - 5322.150T^{-1} + 131.925\times10^{-3}T$$

1687-2000 K:
$$\Delta Hf° = -627.977 - 0.944\times10^{-3}T + 3.733\times10^{-6}T^{2} - 10545.801T^{-1}$$
$$\Delta Gf° = -627.977 + 0.944\times10^{-3}T\ln T - 3.733\times10^{-6}T^{2} - 5272.900T^{-1} + 136.740\times10^{-3}T$$

Source: Data from Fegley (144) who estimated all above 298 K.

$SrTiO_3(c)$
Strontium Titanate
[Formation: $Sr(c,l,g) + Ti(c) + 1.5O_2(g) = SrTiO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	23.510	26.000	26.000	0	-399.710	-379.636	278.277
300	23.564	26.146	26.000	.044	-399.708	-379.510	276.469
400	25.710	33.244	26.954	2.516	-399.577	-372.795	203.683
500	27.064	39.136	28.818	5.159	-399.372	-366.123	160.030
600	28.013	44.159	30.966	7.916	-399.154	-359.494	130.944
700	28.708	48.532	33.171	10.753	-398.964	-352.894	110.177
800	29.222	52.401	35.337	13.651	-398.823	-346.327	94.611
828	29.328	53.408	35.931	14.471	-398.796	-344.490	90.927
828	29.328	53.408	35.931	14.471	-398.976	-344.490	90.927
900	29.599	55.865	37.428	16.593	-398.918	-339.752	82.502
1000	29.869	58.999	39.432	19.567	-398.842	-333.181	72.816
1041	29.946	60.201	40.226	20.793	-398.817	-330.489	69.383
1041	29.946	60.201	40.226	20.793	-400.777	-330.489	69.383
1100	30.057	61.855	41.342	22.564	-400.711	-326.513	64.871
1156	30.128	63.349	42.372	24.250	-400.653	-322.733	61.014
1156	30.128	63.349	42.372	24.250	-401.670	-322.733	61.014
1200	30.184	64.476	43.162	25.577	-401.585	-319.730	58.230
1300	30.268	66.896	44.896	28.600	-401.406	-312.917	52.606
1400	30.330	69.141	46.548	31.630	-401.253	-306.116	47.786
1500	30.386	71.236	48.126	34.665	-401.123	-299.327	43.611
1600	30.454	73.199	49.632	37.707	-401.019	-292.543	39.959
1654.1	30.506	74.212	50.420	39.356	-400.972	-288.876	38.168
1654.1	30.506	74.212	50.420	39.356	-433.702	-288.876	38.168
1700	30.551	75.048	51.073	40.757	-433.512	-284.861	36.621
1800	30.694	76.798	52.454	43.819	-433.116	-276.127	33.526

Phase changes:
828 K, α − β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1156 K, α − β transition point of Ti; ΔH° = 1.017 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K:
$Cp° = 28.545 + 1.490\times10^{-3}T - 4.871\times10^{5}T^{-2}$
$H°-H°_{298} = 28.545\times10^{-3}T + 0.745\times10^{-6}T^{2} + 4.871\times10^{2}T^{-1} - 10.211$

Formation equations (kcal/mol):

298.15-828 K:
$ΔHf° = -403.102 + 7.629\times10^{-3}T - 3.665\times10^{-6}T^{2} + 430.200T^{-1}$
$ΔGf° = -403.102 - 7.629\times10^{-3}T\ln T + 3.665\times10^{-6}T^{2} + 215.100T^{-1} + 118.658\times10^{-3}T$

828-1041 K:
$ΔHf° = -401.338 + 3.223\times10^{-3}T - 1.133\times10^{-6}T^{2} + 404.500T^{-1}$
$ΔGf° = -401.338 - 3.223\times10^{-3}T\ln T + 1.133\times10^{-6}T^{2} + 202.250T^{-1} + 89.040\times10^{-3}T$

1041-1156 K:
$ΔHf° = -403.923 + 3.823\times10^{-3}T - 1.133\times10^{-6}T^{2} + 404.500T^{-1}$
$ΔGf° = -403.923 - 3.823\times10^{-3}T\ln T + 1.133\times10^{-6}T^{2} + 202.250T^{-1} + 95.691\times10^{-3}T$

1156-1654.1 K:
$ΔHf° = -407.960 + 6.223\times10^{-3}T - 1.456\times10^{-6}T^{2} + 1187.400T^{-1}$
$ΔGf° = -407.960 - 6.223\times10^{-3}T\ln T + 1.456\times10^{-6}T^{2} + 593.700T^{-1} + 115.444\times10^{-3}T$

1654.1-1800 K:
$ΔHf° = -436.837 + 4.350\times10^{-3}T - 0.480\times10^{-6}T^{2} - 4473.300T^{-1}$
$ΔGf° = -436.837 - 4.350\times10^{-3}T\ln T + 0.480\times10^{-6}T^{2} - 2236.650T^{-1} + 121.668\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Todd (497). High-temperature data based on Coughlin (103).

Sr_2TiO_4(c)
Distrontium Titanate
[Formation: $2Sr(c,l,g) + Ti(c) + 2O_2(g) = Sr_2TiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	34.140	38.000	38.000	0	-547.700	-520.172	381.291
300	34.210	38.211	38.001	.063	-547.698	-520.000	378.815
400	36.864	48.459	39.379	3.632	-547.483	-510.795	279.082
500	38.404	56.863	42.061	7.401	-547.217	-501.656	219.271
600	39.479	63.964	45.136	11.297	-546.979	-492.567	179.415
700	40.313	70.115	48.275	15.288	-546.815	-483.508	150.956
800	40.996	75.544	51.350	19.355	-546.753	-474.473	129.618
828	41.158	76.957	52.192	20.505	-546.757	-471.943	124.567
828	41.158	76.957	52.192	20.505	-547.117	-471.943	124.567
900	41.575	80.407	54.314	23.484	-547.144	-465.403	113.014
1000	42.072	84.814	57.147	27.667	-547.173	-456.317	99.727
1041	42.248	86.508	58.270	29.396	-547.186	-452.591	95.017
1041	42.248	86.508	58.270	29.396	-551.106	-452.591	95.017
1100	42.501	88.844	59.848	31.896	-551.053	-447.015	88.813
1156	42.707	90.961	61.305	34.282	-551.003	-441.717	83.509
1156	42.707	90.961	61.305	34.282	-552.020	-441.717	83.509
1200	42.869	92.559	62.421	36.165	-551.935	-437.520	79.682
1300	43.182	96.003	64.874	40.468	-551.745	-427.994	71.951
1400	43.442	99.213	67.213	44.800	-551.562	-418.481	65.327
1500	43.653	102.217	69.447	49.155	-551.387	-408.982	59.588
1600	43.815	105.040	71.584	53.529	-551.229	-399.491	54.567
1654.1	43.877	106.498	72.702	55.902	-551.151	-394.362	52.105
1654.1	43.877	106.498	72.702	55.902	-616.611	-394.362	52.105
1700	43.930	107.700	73.631	57.917	-616.239	-388.203	49.906
1800	43.998	110.213	75.595	62.313	-615.451	-374.811	45.508

Phase changes: 828 K, α − β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1156 K, α − β transition point of Ti; ΔH° = 1.017 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 38.978 + 3.364\times10^{-3}T - 5.192\times10^{5}T^{-2}$
$H°-H°_{298} = 38.978\times10^{-3}T + 1.682\times10^{-6}T^{2} + 5.192\times10^{2}T^{-1} - 13.512$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf° = -551.709 + 9.853\times10^{-3}T - 5.511\times10^{-6}T^{2} + 465.400T^{-1}$
$\Delta Gf° = -551.709 - 9.853\times10^{-3}T\ln T + 5.511\times10^{-6}T^{2} + 232.700T^{-1} + 157.653\times10^{-3}T$
828-1041 K: $\Delta Hf° = -548.182 + 1.041\times10^{-3}T - 0.447\times10^{-6}T^{2} + 414.000T^{-1}$
$\Delta Gf° = -548.182 - 1.041\times10^{-3}T\ln T + 0.447\times10^{-6}T^{2} + 207.000T^{-1} + 98.417\times10^{-3}T$
1041-1156 K: $\Delta Hf° = -553.351 + 2.241\times10^{-3}T - 0.447\times10^{-6}T^{2} + 414.000T^{-1}$
$\Delta Gf° = -553.351 - 2.241\times10^{-3}T\ln T + 0.447\times10^{-6}T^{2} + 207.000T^{-1} + 111.720\times10^{-3}T$
1156-1654.1 K: $\Delta Hf° = -557.388 + 4.641\times10^{-3}T - 0.770\times10^{-6}T^{2} + 1196.900T^{-1}$
$\Delta Gf° = -557.388 - 4.641\times10^{-3}T\ln T + 0.770\times10^{-6}T^{2} + 598.450T^{-1} + 131.472\times10^{-3}T$
1654.1-1800 K: $\Delta Hf° = -615.143 + 0.895\times10^{-3}T + 1.180\times10^{-6}T^{2} - 10124.500T^{-1}$
$\Delta Gf° = -615.143 - 0.895\times10^{-3}T\ln T - 1.180\times10^{-6}T^{2} - 5062.250T^{-1} + 143.921\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from Todd (497). High-temperature data based on Coughlin (103).

$SrZrO_3(c)$
Strontium Zirconate
[Formation: $Sr(c,l,g) + Zr(c) + 1.5O_2(g) = SrZrO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	24.710	27.500	27.500	0	-422.400	-402.177	294.800
300	24.820	27.650	27.500	.050	-422.393	-402.046	292.887
400	28.790	35.440	28.540	2.760	-422.046	-395.317	215.988
500	30.550	42.080	30.600	5.740	-421.529	-388.690	169.894
600	31.500	47.740	32.990	8.850	-420.985	-382.170	139.204
700	32.070	52.640	35.454	12.030	-420.477	-375.741	117.310
800	32.440	56.950	37.888	15.250	-420.036	-369.392	100.912
828	32.507	58.067	38.551	16.159	-419.925	-367.622	97.032
828	32.507	58.067	38.551	16.159	-420.105	-367.622	97.032
900	32.680	60.780	40.213	18.510	-419.828	-363.060	88.162
1000	32.860	64.240	42.450	21.790	-419.464	-356.776	77.972
1041	32.909	65.561	43.334	23.138	-419.322	-354.208	74.362
1041	32.909	65.561	43.334	23.138	-421.282	-354.208	74.362
1100	32.980	67.370	44.570	25.080	-421.051	-350.406	69.618
1136	33.012	68.433	45.309	26.268	-420.912	-348.097	66.968
1136	33.012	68.433	45.309	26.268	-421.863	-348.097	66.968
1200	33.070	70.250	46.600	28.380	-421.535	-343.959	62.643
1300	33.140	72.900	48.523	31.690	-421.036	-337.517	56.741
1400	33.190	75.360	50.353	35.010	-420.554	-331.109	51.688
1500	33.230	77.650	52.097	38.330	-420.099	-324.737	47.314
1600	33.260	79.790	53.753	41.660	-419.659	-318.378	43.488
1654.1	33.276	80.899	54.630	43.452	-419.440	-314.970	41.615
1654.1	33.276	80.899	54.630	43.452	-452.170	-314.970	41.615
1700	33.290	81.810	55.351	44.980	-451.827	-311.169	40.003
1800	33.310	83.720	56.881	48.310	-451.094	-302.927	36.780
1900	33.320	85.520	58.336	51.650	-450.378	-294.704	33.898
2000	33.330	87.230	59.740	54.980	-449.697	-286.533	31.311

Phase changes: 828 K, α – β transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1136 K, α – β transition point of Zr; ΔH° = 0.951 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2400 K: $Cp° = 33.762 - 0.118\times10^{-3}T - 7.877\times10^{5}T^{-2}$
$H°-H°_{298} = 33.762\times10^{-3}T - 0.059\times10^{-6}T^{2} + 7.877\times10^{2}T^{-1} - 12.703$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf° = -428.085 + 12.330\times10^{-3}T - 4.287\times10^{-6}T^{2} + 712.700T^{-1}$
$\Delta Gf° = -428.085 - 12.330\times10^{-3}T\ln T + 4.287\times10^{-6}T^{2} + 356.350T^{-1} + 151.861\times10^{-3}T$
828-1041 K: $\Delta Hf° = -426.322 + 7.924\times10^{-3}T - 1.756\times10^{-6}T^{2} + 687.000T^{-1}$
$\Delta Gf° = -426.322 - 7.924\times10^{-3}T\ln T + 1.756\times10^{-6}T^{2} + 343.500T^{-1} + 122.243\times10^{-3}T$
1041-1136 K: $\Delta Hf° = -428.907 + 8.524\times10^{-3}T - 1.756\times10^{-6}T^{2} + 687.000T^{-1}$
$\Delta Gf° = -428.907 - 8.524\times10^{-3}T\ln T + 1.756\times10^{-6}T^{2} + 343.500T^{-1} + 128.894\times10^{-3}T$
1136-1654.1 K: $\Delta Hf° = -431.403 + 9.693\times10^{-3}T - 1.625\times10^{-6}T^{2} + 741.500T^{-1}$
$\Delta Gf° = -431.403 - 9.693\times10^{-3}T\ln T + 1.625\times10^{-6}T^{2} + 370.750T^{-1} + 139.443\times10^{-3}T$
1654.1-2000 K: $\Delta Hf° = -460.280 + 7.820\times10^{-3}T - 0.650\times10^{-6}T^{2} - 4919.200T^{-1}$
$\Delta Gf° = -460.280 - 7.820\times10^{-3}T\ln T + 0.650\times10^{-6}T^{2} - 2459.600T^{-1} + 145.668\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (391). Low-temperature heat capacities and entropy at 298 K from King (270). High-temperature data based on Fomichev (154) and Nagarajan (346).

$TaB_2(c)$
Tantalum Diboride
[Formation: $Ta(c) + 2B(\beta,l) = TaB_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.500	10.603	10.603	0	-45.000	-44.363	32.518
300	11.559	10.674	10.604	.021	-45.000	-44.356	32.313
400	13.759	14.337	11.087	1.300	-44.971	-44.151	24.122
500	15.019	17.553	12.067	2.743	-44.967	-43.942	19.207
600	15.908	20.373	13.221	4.291	-44.999	-43.740	15.932
700	16.623	22.881	14.425	5.919	-45.043	-43.523	13.588
800	17.245	25.142	15.626	7.613	-45.083	-43.301	11.829
900	17.813	27.206	16.799	9.366	-45.116	-43.077	10.460
1000	18.347	29.111	17.937	11.174	-45.138	-42.848	9.364
1100	18.859	30.883	19.033	13.035	-45.145	-42.629	8.470
1200	19.356	32.546	20.091	14.946	-45.138	-42.397	7.721
1300	19.842	34.114	21.109	16.906	-45.119	-42.161	7.088
1400	20.321	35.602	22.092	18.914	-45.088	-41.937	6.547
1500	20.794	37.020	23.040	20.970	-45.048	-41.705	6.076
1600	21.263	38.377	23.957	23.072	-45.001	-41.508	5.670
1700	21.728	39.680	24.844	25.222	-44.943	-41.290	5.308
1800	22.191	40.935	25.703	27.418	-44.876	-41.053	4.984
1900	22.652	42.148	26.537	29.660	-44.802	-40.840	4.698
2000	23.111	43.321	27.347	31.948	-44.721	-40.661	4.443
2100	23.569	44.460	28.135	34.282	-44.634	-40.438	4.208
2200	24.026	45.567	28.902	36.662	-44.542	-40.261	3.999
2300	24.482	46.645	29.650	39.088	-44.446	-40.044	3.805
2350	24.710	47.174	30.018	40.318	-44.396	-39.984	3.718
2350	24.710	47.174	30.018	40.318	-68.396	-39.984	3.718
2400	24.937	47.697	30.381	41.559	-68.303	-39.361	3.584
2500	25.391	48.724	31.094	44.075	-68.095	-38.190	3.339
2600	25.845	49.728	31.791	46.637	-67.860	-36.967	3.107
2700	26.298	50.712	32.473	49.244	-67.600	-35.799	2.898
2800	26.751	51.677	33.143	51.896	-67.318	-34.645	2.704
2900	27.204	52.624	33.798	54.594	-67.016	-33.443	2.520
3000	27.656	53.553	34.441	57.337	-66.702	-32.313	2.354

*Entropy at 298 K estimated.

Phase change: 2350 K, melting point of B; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 14.213 + 4.494\times10^{-3}T - 3.603\times10^{5}T^{-2}$

$H°-H°_{298} = 14.213\times10^{-3}T + 2.247\times10^{-6}T^{2} + 3.603\times10^{2}T^{-1} - 5.646$

Formation equations (kcal/mol):

298.15-2350 K: $\Delta Hf° = -44.831 - 0.289\times10^{-3}T + 0.181\times10^{-6}T^{2} - 29.500T^{-1}$

$\Delta Gf° = -44.831 + 0.289\times10^{-3}T\ln T - 0.181\times10^{-6}T^{2} - 14.750T^{-1} + 0.143\times10^{-3}T$

2350-3000 K: $\Delta Hf° = -63.611 - 5.843\times10^{-3}T + 1.565\times10^{-6}T^{2} + 413.500T^{-1}$

$\Delta Gf° = -63.611 + 5.843\times10^{-3}T\ln T - 1.565\times10^{-6}T^{2} + 206.750T^{-1} - 31.764\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kirpichev (273). Other data from Schick (437) who estimated entropy at 298 K.

$TaC(c)$
Tantalum Carbide
[Formation: $Ta(c) + C(c) = TaC(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	8.793	10.127	10.127	0	-34.440	-34.093	24.990
300	8.820	10.182	10.129	.016	-34.439	-34.090	24.834
400	9.958	12.886	10.488	.959	-34.356	-33.986	18.569
500	10.643	15.186	11.204	1.991	-34.266	-33.904	14.819
600	11.101	17.168	12.036	3.079	-34.185	-33.838	12.325
700	11.446	18.906	12.896	4.207	-34.117	-33.787	10.549
800	11.729	20.454	13.747	5.366	-34.059	-33.744	9.218
900	11.978	21.850	14.571	6.551	-34.009	-33.709	8.186
1000	12.205	23.124	15.363	7.761	-33.960	-33.678	7.360
1100	12.411	24.297	16.122	8.992	-33.913	-33.641	6.684
1200	12.614	25.385	16.849	10.243	-33.866	-33.628	6.124
1300	12.815	26.403	17.546	11.514	-33.818	-33.611	5.651
1400	13.012	27.360	18.213	12.806	-33.766	-33.598	5.245
1500	13.206	28.264	18.853	14.117	-33.713	-33.587	4.894
1600	13.393	29.122	19.468	15.447	-33.656	-33.579	4.587
1700	13.579	29.940	20.061	16.795	-33.598	-33.579	4.317
1800	13.764	30.721	20.631	18.162	-33.535	-33.578	4.077
1900	13.948	31.470	21.182	19.548	-33.469	-33.581	3.863
2000	14.132	32.190	21.714	20.952	-33.402	-33.590	3.670
2100	14.314	32.884	22.230	22.374	-33.333	-33.602	3.497
2200	14.496	33.554	22.729	23.815	-33.262	-33.616	3.339
2300	14.677	34.203	23.215	25.273	-33.192	-33.634	3.196
2400	14.858	34.831	23.685	26.750	-33.122	-33.655	3.065
2500	15.039	35.441	24.143	28.245	-33.052	-33.677	2.944

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 10.577 + 1.808x10^{-3}T - 2.065x10^{5}T^{-2}$
$H°- H°_{298} = 10.577x10^{-3}T + 0.904x10^{-6}T^{2} + 2.065x10^{2}T^{-1} - 3.926$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -35.282 + 2.003x10^{-3}T - 0.544x10^{-6}T^{2} + 87.400T^{-1}$
$\Delta Gf° = -35.282 - 2.003x10^{-3}T\ln T + 0.544x10^{-6}T^{2} + 43.700T^{-1} + 14.747x10^{-3}T$
2000-2500 K: $\Delta Hf° = -33.290 - 0.120x10^{-3}T + 0.088x10^{-6}T^{2} - 460.300T^{-1}$
$\Delta Gf° = -33.290 + 0.120x10^{-3}T\ln T - 0.088x10^{-6}T^{2} - 230.150T^{-1} - 1.053x10^{-3}T$

Source: Data from Chase (83).

$Ta_2C(c)$
Ditantalum Carbide
[Formation: $2Ta(c) + C(c) = Ta_2C(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.567	20.700	20.700	0	-51.000	-50.847	37.272
300	14.601	20.790	20.700	.027	-50.999	-50.845	37.040
400	15.931	25.193	21.291	1.561	-50.941	-50.803	27.757
500	16.725	28.839	22.447	3.196	-50.873	-50.776	22.194
600	17.309	31.942	23.777	4.899	-50.807	-50.761	18.490
700	17.793	34.648	25.141	6.655	-50.747	-50.760	15.848
800	18.224	37.052	26.482	8.456	-50.689	-50.765	13.868
900	18.624	39.222	27.780	10.298	-50.630	-50.780	12.331
1000	19.005	41.204	29.024	12.180	-50.563	-50.800	11.102
1100	19.374	43.033	30.216	14.099	-50.488	-50.817	10.096
1200	19.734	44.734	31.356	16.054	-50.403	-50.860	9.263
1300	20.088	46.327	32.445	18.046	-50.307	-50.900	8.557
1400	20.437	47.829	33.492	20.072	-50.202	-50.952	7.954
1500	20.784	49.251	34.496	22.133	-50.089	-51.010	7.432
1600	21.128	50.603	35.460	24.229	-49.965	-51.074	6.976
1700	21.470	51.894	36.389	26.358	-49.834	-51.150	6.576
1800	21.811	53.131	37.285	28.523	-49.690	-51.229	6.220
1900	22.150	54.319	38.150	30.721	-49.540	-51.317	5.903
2000	22.489	55.464	38.988	32.953	-49.384	-51.418	5.619

*Data except enthalpy of formation and entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 15.880 + 3.330\times10^{-3}T - 2.050\times10^{5}T^{-2}$

$H°-H°_{298} = 15.880\times10^{-3}T + 1.665\times10^{-6}T^{2} + 2.050\times10^{2}T^{-1} - 5.570$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -52.096 + 2.250\times10^{-3}T - 0.465\times10^{-6}T^{2} + 139.100T^{-1}$

$\Delta Gf° = -52.096 - 2.250\times10^{-3}T\ln T + 0.465\times10^{-6}T^{2} + 69.550T^{-1} + 16.087\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (515). Other data are those estimated by Schick (437).

TaN(c)
Tantalum Nitride
[Formation: $Ta(c) + 0.5N_2(g) = TaN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	10.000	10.000	10.000	0	-60.100	-53.301	39.070
300	10.020	10.060	10.000	.020	-60.097	-53.256	38.796
400	10.570	13.020	10.395	1.050	-60.032	-50.985	27.857
500	10.950	15.420	11.160	2.130	-59.928	-48.730	21.300
600	11.240	17.450	12.050	3.240	-59.805	-46.506	16.940
700	11.500	19.200	12.957	4.370	-59.674	-44.306	13.833
800	11.730	20.750	13.825	5.540	-59.518	-42.112	11.504
900	11.950	22.150	14.683	6.720	-59.365	-39.954	9.702
1000	12.170	23.420	15.490	7.930	-59.197	-37.802	8.262
1100	12.380	24.590	16.272	9.150	-59.031	-35.679	7.089
1200	12.590	25.670	17.003	10.400	-58.847	-33.554	6.111
1300	12.790	26.690	17.713	11.670	-58.656	-31.458	5.288
1400	12.990	27.640	18.383	12.960	-58.457	-29.366	4.584
1500	13.200	28.550	19.037	14.270	-58.251	-27.304	3.978
1600	13.400	29.410	19.660	15.600	-58.039	-25.251	3.449
1700	13.600	30.220	20.249	16.950	-57.818	-23.195	2.982
1800	13.790	31.010	20.832	18.320	-57.589	-21.177	2.571

*Entropy and heat capacity at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 10.286 + 1.966 \times 10^{-3}T - 0.798 \times 10^{5}T^{-2}$

$H°-H°_{298} = 10.286 \times 10^{-3}T + 0.983 \times 10^{-6}T^{2} + 0.798 \times 10^{2}T^{-1} - 3.422$

Formation equations (kcal/mol):

298.15-1800 K: $\Delta Hf° = -61.148 + 1.972 \times 10^{-3}T + 0.007 \times 10^{-6}T^{2} + 136.950T^{-1}$

$\Delta Gf° = -61.148 - 1.972 \times 10^{-3}T\ln T - 0.007 \times 10^{-6}T^{2} + 68.475T^{-1} + 36.783 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Entropy and heat capacity at 298 K estimated. High-temperature data based on Bolgar (48).

$Ta_2N(c)$
Ditantalum Nitride
[Formation: $2Ta(c) + 0.5N_2(g) = Ta_2N(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	15.500	15.000	15.000	0	-65.000	-56.734	41.586
300	15.520	15.100	15.000	.030	-64.999	-56.681	41.291
400	16.520	19.700	15.625	1.630	-64.979	-53.913	29.456
500	17.380	23.480	16.820	3.330	-64.881	-51.151	22.358
600	18.180	26.720	18.203	5.110	-64.717	-48.417	17.636
700	18.950	29.580	19.637	6.960	-64.503	-45.724	14.275
800	19.700	32.160	21.035	8.900	-64.218	-43.052	11.761
900	20.450	34.530	22.419	10.900	-63.894	-40.440	9.820
1000	21.190	36.720	23.730	12.990	-63.499	-37.843	8.270
1100	21.930	38.770	25.006	15.140	-63.063	-35.300	7.013
1200	22.660	40.710	26.235	17.370	-62.565	-32.796	5.973
1300	23.390	42.560	27.429	19.670	-62.017	-30.348	5.102
1400	24.120	44.320	28.570	22.050	-61.409	-27.932	4.360
1500	24.860	46.010	29.677	24.500	-60.754	-25.563	3.724
1600	25.590	47.630	30.743	27.020	-60.049	-23.230	3.173
1700	26.310	49.210	31.786	29.620	-59.287	-20.960	2.695
1800	27.040	50.730	32.797	32.280	-58.485	-18.727	2.274
1900	27.770	52.210	33.778	35.020	-57.628	-16.537	1.902
2000	28.500	53.660	34.740	37.840	-56.715	-14.410	1.575
2100	29.230	55.060	35.670	40.720	-55.767	-12.305	1.281
2200	29.960	56.440	36.585	43.680	-54.768	-10.266	1.020

*Entropy and heat capacity at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2200 K: $Cp^\circ = 13.979 + 7.268\times10^{-3}T - 0.580\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 13.979\times10^{-3}T + 3.634\times10^{-6}T^2 + 0.580\times10^{2}T^{-1} - 4.685$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -65.922 + 0.608\times10^{-3}T + 1.975\times10^{-6}T^2 + 168.350T^{-1}$
$\Delta Gf^\circ = -65.922 - 0.608\times10^{-3}T\ln T - 1.975\times10^{-6}T^2 + 84.175T^{-1} + 33.925\times10^{-3}T$
2000-2200 K: $\Delta Hf^\circ = -64.585 - 0.456\times10^{-3}T + 2.242\times10^{-6}T^2 - 381.600T^{-1}$
$\Delta Gf^\circ = -64.585 + 0.456\times10^{-3}T\ln T - 2.242\times10^{-6}T^2 - 190.800T^{-1} + 25.771\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Entropy and heat capacity at 298 K estimated. High-temperature data based on Bolgar (48).

$TaOCl_3(g)$
Tantalum Oxide Trichloride (ideal gas)
[Formation: Ta(c) + 1.5Cl_2(g) + 0.5O_2(g) = $TaOCl_3$(g)]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	21.954	86.243	86.243	0	-186.600	-178.218	130.635
300	21.984	86.379	86.243	.041	-186.599	-178.164	129.791
400	23.237	92.891	87.121	2.308	-186.548	-175.360	95.811
500	23.990	98.164	88.820	4.672	-186.454	-172.573	75.430
600	24.469	102.583	90.755	7.097	-186.340	-169.806	61.851
700	24.789	106.381	92.724	9.560	-186.219	-167.061	52.158
800	25.011	109.706	94.642	12.051	-186.098	-164.334	44.893
900	25.171	112.662	96.483	14.561	-185.978	-161.619	39.246
1000	25.289	115.320	98.236	17.084	-185.864	-158.921	34.732
1100	25.379	117.735	99.900	19.618	-185.755	-156.231	31.040
1200	25.448	119.946	101.480	22.159	-185.654	-153.551	27.965
1300	25.503	121.985	102.980	24.707	-185.560	-150.879	25.365
1400	25.547	123.877	104.406	27.259	-185.477	-148.216	23.137
1500	25.583	125.641	105.764	29.816	-185.404	-145.558	21.207
1600	25.612	127.293	107.058	32.376	-185.343	-142.903	19.519
1700	25.637	128.846	108.294	34.938	-185.294	-140.249	18.030
1800	25.658	130.312	109.477	37.503	-185.256	-137.602	16.707
1900	25.675	131.700	110.611	40.069	-185.233	-134.953	15.523
2000	25.690	133.017	111.699	42.636	-185.227	-132.311	14.458

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 24.860 + 0.594\times10^{-3}T - 2.740\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.860\times10^{-3}T + 0.297\times10^{-6}T^{2} + 2.740\times10^{2}T^{-1} - 8.357$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -188.089 + 2.949\times10^{-3}T - 0.769\times10^{-6}T^{2} + 202.150T^{-1}$

$\Delta Gf^\circ = -188.089 - 2.949\times10^{-3}T\ln T + 0.769\times10^{-6}T^{2} + 101.075T^{-1} + 48.541\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Other data are those estimated by Zavalishin (541).

$TaOF_3(g)$
Tantalum Oxide Trifluoride (ideal gas)

[Formation: $Ta(c) + 1.5F_2(g) + 0.5O_2(g) = TaOF_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	19.580	77.900	77.900	0	-310.000	-301.298	220.854
300	19.620	78.030	77.900	.039	-310.000	-301.243	219.453
400	21.470	83.940	78.690	2.100	-310.063	-298.310	162.987
500	22.670	88.870	80.250	4.310	-310.049	-295.373	129.106
600	23.480	93.080	82.045	6.621	-309.991	-292.442	106.521
700	24.020	96.750	83.896	8.998	-309.911	-289.528	90.394
800	24.400	99.980	85.705	11.420	-309.823	-286.621	78.300
900	24.680	102.900	87.489	13.870	-309.734	-283.756	68.904
1000	24.890	105.500	89.150	16.350	-309.642	-280.863	61.382
1100	25.050	107.900	90.764	18.850	-309.551	-278.008	55.234
1200	25.160	110.100	92.300	21.360	-309.467	-275.163	50.113
1300	25.260	112.100	93.731	23.880	-309.391	-272.284	45.775
1400	25.330	113.900	95.036	26.410	-309.323	-269.330	42.044
1500	25.400	115.700	96.400	28.950	-309.263	-266.547	38.835
1600	25.450	117.300	97.619	31.490	-309.220	-263.638	36.011
1700	25.490	118.900	98.882	34.030	-309.190	-260.891	33.539
1800	25.530	120.300	99.972	36.590	-309.160	-257.937	31.317
1900	25.570	121.700	101.089	39.160	-309.134	-255.110	29.344
2000	25.580	123.000	102.155	41.690	-309.168	-252.274	27.567

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 23.998 + 1.098\times10^{-3}T - 4.218\times10^{5}T^{-2}$

$H°-H°_{298} = 23.998\times10^{-3}T + 0.549\times10^{-6}T^{2} + 4.218\times10^{2}T^{-1} - 8.619$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -311.719 + 2.565\times10^{-3}T - 0.646\times10^{-6}T^{2} + 301.650T^{-1}$

$\Delta Gf° = -311.719 - 2.565\times10^{-3}T\ln T + 0.646\times10^{-6}T^{2} + 150.825T^{-1} + 47.678\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Rakov (414). Other data from Mendeleeva (330).

TaSi$_2$(c)
Tantalum Disilicide
[Formation: Ta(c) + 2Si(c,l) = TaSi$_2$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	15.630	18.000	18.000	0	-28.500	-28.226	20.690
300	15.650	18.100	18.003	.029	-28.500	-28.224	20.561
400	16.890	22.800	18.675	1.650	-28.509	-28.154	15.382
500	17.550	26.640	19.860	3.390	-28.486	-28.044	12.258
600	18.000	29.880	21.280	5.160	-28.490	-27.967	10.187
700	18.360	32.700	22.714	6.990	-28.478	-27.882	8.705
800	18.660	35.160	24.097	8.850	-28.470	-27.775	7.588
900	18.900	37.380	25.480	10.710	-28.498	-27.713	6.730
1000	19.140	39.360	26.730	12.630	-28.488	-27.567	6.025
1100	19.350	41.220	27.993	14.550	-28.502	-27.523	5.468
1200	19.560	42.900	29.150	16.500	-28.506	-27.414	4.993
1300	19.770	44.460	30.268	18.450	-28.529	-27.321	4.593
1400	19.980	45.960	31.367	20.430	-28.544	-27.266	4.256
1500	20.190	47.340	32.380	22.440	-28.550	-27.186	3.961
1600	20.370	48.630	33.330	24.480	-28.545	-27.057	3.696
1687	20.553	49.732	34.170	26.253	-28.560	-26.973	3.494
1687	20.553	49.732	34.170	26.253	-52.724	-26.973	3.494
1700	20.580	49.890	34.290	26.520	-52.707	-26.767	3.441
1800	20.760	51.060	35.177	28.590	-52.574	-25.216	3.062
1900	20.940	52.200	36.047	30.690	-52.422	-23.707	2.727
2000	21.150	53.280	36.885	32.790	-52.281	-22.219	2.428

*Entropy at 298 K estimated.

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 17.511 + 1.842\text{x}10^{-3}T - 2.168\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.511\text{x}10^{-3}T + 0.921\text{x}10^{-6}T^2 + 2.168\text{x}10^{2}T^{-1} - 6.030$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf^\circ = -29.031 + 1.097\text{x}10^{-3}T - 0.463\text{x}10^{-6}T^2 + 73.000T^{-1}$
$\Delta Gf^\circ = -29.031 - 1.097\text{x}10^{-3}T\ln T + 0.463\text{x}10^{-6}T^2 + 36.500T^{-1} + 8.402\text{x}10^{-3}T$
1687-2000 K: $\Delta Hf^\circ = -53.889 + 0.255\text{x}10^{-3}T + 0.239\text{x}10^{-6}T^2 + 270.000T^{-1}$
$\Delta Gf^\circ = -53.889 - 0.255\text{x}10^{-3}T\ln T - 0.239\text{x}10^{-6}T^2 + 135.000T^{-1} + 18.030\text{x}10^{-3}T$

Source: Data from Chart (76) who estimated entropy at 298 K.

$TbFeO_3$(c)
Terbium Ferrite
[Formation: Tb(c) + Fe(c) + 1.5O_2(g) = $TbFeO_3$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	25.098	26.500	26.500	0	-324.600	-303.417	222.408
300	25.167	26.655	26.502	.046	-324.598	-303.287	220.941
400	27.910	34.311	27.526	2.714	-324.306	-296.222	161.846
500	29.479	40.722	29.542	5.590	-323.888	-289.252	126.430
600	30.422	46.188	31.873	8.589	-323.455	-282.364	102.850
700	30.972	50.923	34.263	11.662	-323.077	-275.545	86.028

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = 28.692 + 4.998\text{x}10^{-3}T - 4.519\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 28.692\text{x}10^{-3}T + 2.499\text{x}10^{-6}T^{2} + 4.519\text{x}10^{2}T^{-1} - 10.292$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -330.599 + 13.784\text{x}10^{-3}T - 6.441\text{x}10^{-6}T^{2} + 734.000T^{-1}$

$\Delta Gf^\circ = -330.599 - 13.784\text{x}10^{-3}T\ln T + 6.441\text{x}10^{-6}T^{2} + 367.000T^{-1} + 163.655\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kaul (237). Other data based on Shchelkotunov (443).

TbO(g)
Terbium Monoxide (ideal gas)
[Formation: $Tb(c,l) + 0.5O_2(g) = TbO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.550	61.711	61.711	0	-17.000	-22.870	16.764
300	7.560	61.758	61.711	.014	-17.006	-22.908	16.688
400	7.940	63.987	62.012	.790	-17.269	-24.834	13.569
500	8.210	65.789	62.593	1.598	-17.507	-26.701	11.671
600	8.390	67.303	63.255	2.429	-17.750	-28.516	10.387
700	8.520	68.606	63.929	3.274	-18.027	-30.289	9.457
800	8.610	69.751	64.587	4.131	-18.336	-32.016	8.746
900	8.670	70.768	65.218	4.995	-18.680	-33.708	8.185
1000	8.720	71.685	65.820	5.865	-19.063	-35.363	7.728
1100	8.750	72.516	66.391	6.738	-19.485	-36.965	7.344
1200	8.780	73.280	66.934	7.615	-19.946	-38.541	7.019
1300	8.800	73.985	67.450	8.495	-20.453	-40.068	6.736
1400	8.820	74.637	67.940	9.376	-21.010	-41.549	6.486
1500	8.840	75.246	68.407	10.259	-21.621	-42.995	6.264
1560	8.846	75.594	68.677	10.790	-22.016	-43.849	6.143
1560	8.846	75.594	68.677	10.790	-23.216	-43.849	6.143
1600	8.850	75.818	68.853	11.144	-23.303	-44.373	6.061
1630	8.853	75.982	68.983	11.410	-23.370	-44.775	6.003
1630	8.853	75.982	68.983	11.410	-25.950	-44.775	6.003
1700	8.860	76.354	69.278	12.029	-26.419	-45.573	5.859
1800	8.870	76.861	69.686	12.915	-27.087	-46.689	5.669
1900	8.880	77.341	70.076	13.803	-27.757	-47.761	5.494
2000	8.880	77.797	70.451	14.691	-28.430	-48.797	5.332

*Data except enthalpy of formation at 298 K estimated.

Phase Changes: 1560 K, α - β transition point of Tb; ΔH° = 1.200 kcal/mol.
1630 K, melting point of Tb; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.443 + 0.304\times10^{-3}T - 0.874\times10^{5}T^{-2}$
$H°- H°_{298} = 8.443\times10^{-3}T + 0.152\times10^{-6}T^{2} + 0.874\times10^{2}T^{-1} - 2.824$

Formation equations (kcal/mol):

298.15-1560 K: $\Delta Hf° = -17.590 + 0.544\times10^{-3}T - 2.214\times10^{-6}T^{2} + 186.200T^{-1}$
$\Delta Gf° = -17.590 - 0.544\times10^{-3}T\ln T + 2.214\times10^{-6}T^{2} + 93.100T^{-1} - 16.318\times10^{-3}T$
1560-1630 K: $\Delta Hf° = -20.180 - 1.813\times10^{-3}T - 0.099\times10^{-6}T^{2} + 64.800T^{-1}$
$\Delta Gf° = -20.180 + 1.813\times10^{-3}T\ln T + 0.099\times10^{-6}T^{2} + 32.400T^{-1} - 28.664\times10^{-3}T$
1630-2000 K: $\Delta Hf° = -15.475 - 6.282\times10^{-3}T - 0.099\times10^{-6}T^{2} + 64.800T^{-1}$
$\Delta Gf° = -15.475 + 6.282\times10^{-3}T\ln T + 0.099\times10^{-6}T^{2} + 32.400T^{-1} - 64.605\times10^{-3}T$

Source: Data from Pedley (396) who estimated all except enthalpy of formation at 298 K.

TeO(g)
Tellurium Monoxide (ideal gas)
[Reaction: $0.5Te_2(g) + 0.5O_2(g) = TeO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15	9.000	56.260	56.260	0	-2.665	-2.910	2.133
300	9.020	56.317	56.260	.017	-2.663	-2.912	2.122
400	9.520	58.995	56.622	.949	-2.525	-3.015	1.647
500	9.590	61.132	57.318	1.907	-2.381	-3.154	1.378
600	9.530	62.877	58.104	2.864	-2.257	-3.319	1.209
700	9.450	64.340	58.893	3.813	-2.162	-3.504	1.094
800	9.380	65.597	59.654	4.754	-2.093	-3.703	1.011
900	9.310	66.697	60.377	5.688	-2.047	-3.907	.949
1000	9.270	67.676	61.059	6.617	-2.020	-4.116	.900
1100	9.230	68.556	61.701	7.541	-2.012	-4.323	.859
1200	9.200	69.360	62.308	8.463	-2.019	-4.534	.826
1300	9.180	70.095	62.878	9.382	-2.041	-4.743	.797
1400	9.160	70.774	63.418	10.299	-2.076	-4.949	.773
1500	9.150	71.407	63.930	11.215	-2.118	-5.156	.751
1600	9.140	71.997	64.416	12.130	-2.163	-5.359	.732
1700	9.140	72.551	64.878	13.044	-2.211	-5.550	.713
1800	9.140	73.073	65.319	13.958	-2.261	-5.747	.698
1900	9.140	73.568	65.741	14.872	-2.311	-5.941	.683
2000	9.140	74.037	66.144	15.786	-2.362	-6.130	.670

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 10.210 - 0.716\text{x}10^{-3}T - 0.886\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.210\text{x}10^{-3}T - 0.358\text{x}10^{-6}T^{2} + 0.886\text{x}10^{2}T^{-1} - 3.309$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -3.450 + 2.295\text{x}10^{-3}T - 0.906\text{x}10^{-6}T^{2} + 53.900T^{-1}$

$\Delta Gr^\circ = -3.450 - 2.295\text{x}10^{-3}T\ln T + 0.906\text{x}10^{-6}T^{2} + 26.950T^{-1} + 14.315\text{x}10^{-3}T$

Source: Data from Pedley (396).

$ThC_{1.94}(c)$
Thorium Carbide
[Formation: $Th(c,l) + 1.94C(c) = ThC_{1.94}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.550	16.800	16.800	0	-35.300	-35.711	26.176
300	13.580	16.870	16.800	.025	-35.295	-35.710	26.014
400	14.670	20.960	17.352	1.443	-35.015	-35.898	19.613
500	15.370	24.310	18.416	2.947	-34.813	-36.143	15.798
600	15.890	27.150	19.632	4.511	-34.687	-36.415	13.264
700	16.350	29.640	20.893	6.123	-34.625	-36.714	11.462
800	16.750	31.860	22.136	7.779	-34.605	-37.019	10.113
900	17.160	33.840	23.312	9.475	-34.621	-37.308	9.060
1000	17.520	35.680	24.471	11.209	-34.656	-37.619	8.221
1100	17.900	37.360	25.559	12.981	-34.704	-37.881	7.526
1200	18.260	38.930	26.607	14.788	-34.765	-38.187	6.955
1300	18.620	40.420	27.627	16.631	-34.831	-38.488	6.470
1400	18.950	41.800	28.579	18.509	-34.899	-38.751	6.049
1500	19.310	43.120	29.505	20.423	-34.967	-39.025	5.686
1600	19.650	44.380	30.398	22.371	-35.030	-39.295	5.367
1633	19.765	44.782	30.685	23.021	-35.052	-39.383	5.271
1633	19.765	44.782	30.685	23.021	-35.912	-39.383	5.271
1700	20.000	45.600	31.272	24.354	-35.907	-39.556	5.085
1700	20.000	45.890	31.272	24.854	-35.407	-39.556	5.085
1763	20.000	46.610	31.799	26.114	-35.412	-39.693	4.920
1763	20.000	48.030	31.799	28.614	-32.912	-39.693	4.920
1800	20.000	48.460	32.153	29.353	-32.923	-39.864	4.840
1900	20.000	49.530	33.028	31.353	-32.975	-40.226	4.627
2000	20.000	50.560	33.884	33.353	-33.069	-40.614	4.438
2023	20.000	50.789	34.074	33.813	-33.094	-40.699	4.397
2023	20.000	50.789	34.074	33.813	-36.394	-40.699	4.397
2100	20.000	51.540	34.705	35.353	-36.601	-40.871	4.253
2200	20.000	52.470	35.491	37.353	-36.877	-41.066	4.080
2300	20.000	53.360	36.250	39.353	-37.160	-41.249	3.919
2400	20.000	54.190	36.960	41.353	-37.454	-41.373	3.767
2500	20.000	55.030	37.689	43.353	-37.751	-41.589	3.636

Phase changes:
1633 K, α - β transition point of Th; $\Delta H^\circ = 0.860$ kcal/mol.
1700 K, α - β transition point of $ThC_{1.94}$; $\Delta H^\circ = 0.500$ kcal/mol.
1763 K, β - γ transition point of $ThC_{1.94}$; $\Delta H^\circ = 2.500$ kcal/mol.
2023 K, melting point of Th; $\Delta H^\circ = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1700 K: $C_p^\circ = 14.293 + 3.390\times10^{-3}T - 1.557\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 14.293\times10^{-3}T + 1.695\times10^{-6}T^2 + 1.557\times10^{2}T^{-1} - 4.934$
1700-1763 K: $C_p^\circ = 20.000$
$H^\circ - H^\circ_{298} = 20.000\times10^{-3}T - 9.146$
1763-2500 K: $C_p^\circ = 20.000$
$H^\circ - H^\circ_{298} = 20.000\times10^{-3}T - 6.646$

Formation equations (kcal/mol):

298.15-1633 K: $\Delta Hf^\circ = -35.029 + 1.410\times10^{-3}T - 0.738\times10^{-6}T^2 - 186.462T^{-1}$
$\Delta Gf^\circ = -35.029 - 1.410\times10^{-3}T\ln T + 0.738\times10^{-6}T^2 - 93.231T^{-1} + 6.577\times10^{-3}T$
1633-1700 K: $\Delta Hf^\circ = -38.278 + 3.659\times10^{-3}T - 1.209\times10^{-6}T^2 - 232.062T^{-1}$
$\Delta Gf^\circ = -38.278 - 3.659\times10^{-3}T\ln T + 1.209\times10^{-6}T^2 - 116.031T^{-1} + 24.444\times10^{-3}T$
1700-1763 K: $\Delta Hf^\circ = -42.490 + 9.366\times10^{-3}T - 2.904\times10^{-6}T^2 - 387.762T^{-1}$
$\Delta Gf^\circ = -42.490 - 9.366\times10^{-3}T\ln T + 2.904\times10^{-6}T^2 - 193.881T^{-1} + 66.518\times10^{-3}T$
1763-2000 K: $\Delta Hf^\circ = -39.990 + 9.366\times10^{-3}T - 2.904\times10^{-6}T^2 - 387.762T^{-1}$
$\Delta Gf^\circ = -39.990 - 9.366\times10^{-3}T\ln T + 2.904\times10^{-6}T^2 - 193.881T^{-1} + 65.100\times10^{-3}T$
2000-2023 K: $\Delta Hf^\circ = -36.126 + 5.247\times10^{-3}T - 1.678\times10^{-6}T^2 - 1450.300T^{-1}$
$\Delta Gf^\circ = -36.126 - 5.247\times10^{-3}T\ln T + 1.678\times10^{-6}T^2 - 725.150T^{-1} + 34.448\times10^{-3}T$
2023-2500 K: $\Delta Hf^\circ = -30.708 - 1.944\times10^{-3}T - 0.260\times10^{-6}T^2 - 1396.800T^{-1}$
$\Delta Gf^\circ = -30.708 + 1.944\times10^{-3}T\ln T + 0.260\times10^{-6}T^2 - 698.400T^{-1} - 20.109\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from Besmann (37).

$ThH_2(c)$
Thorium Dihydride
[Formation: $Th(c) + H_2(g) = ThH_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	8.770	12.120	12.120	0	-34.600	-25.105	18.402
300	8.820	12.180	12.127	.016	-34.609	-25.048	18.247
400	11.420	15.080	12.505	1.030	-34.954	-21.802	11.912
500	13.670	17.870	13.294	2.288	-35.082	-18.493	8.083
600	15.460	20.530	14.282	3.749	-35.028	-15.178	5.528
700	16.870	23.030	15.361	5.368	-34.838	-11.888	3.711
800	18.050	25.360	16.466	7.115	-34.543	-8.626	2.357
900	19.030	27.540	17.572	8.971	-34.165	-5.405	1.313
1000	19.890	29.590	18.673	10.917	-33.722	-2.234	.488

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 8.814 + 12.056 \times 10^{-3}T - 3.234 \times 10^{5}T^{-2}$

$H° - H°_{298} = 8.814 \times 10^{-3}T + 6.028 \times 10^{-6}T^{2} + 3.234 \times 10^{2}T^{-1} - 4.248$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -35.025 - 3.700 \times 10^{-3}T + 4.662 \times 10^{-6}T^{2} + 332.000T^{-1}$

$\Delta Gf° = -35.025 + 3.700 \times 10^{-3}T\ln T - 4.662 \times 10^{-6}T^{2} + 166.000T^{-1} + 11.713 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Picard (398). Other data from Flotow (151).

ThN(c)
Thorium Nitride
[Formation: Th(c) + $0.5N_2(g)$ = ThN(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	10.740	13.400	13.400	0	-93.500	-86.868	63.675
300	10.760	13.470	13.403	.020	-93.499	-86.828	63.253
400	11.540	16.680	13.835	1.138	-93.394	-84.618	46.232
500	12.020	19.310	14.674	2.318	-93.253	-82.440	36.034
600	12.390	21.540	15.642	3.539	-93.095	-80.294	29.247
700	12.700	23.470	16.621	4.794	-92.931	-78.171	24.406
800	12.990	25.190	17.591	6.079	-92.763	-76.077	20.783
900	13.250	26.730	18.518	7.391	-92.598	-73.997	17.969
1000	13.510	28.140	19.411	8.729	-92.432	-71.940	15.722
1100	13.750	29.440	20.265	10.092	-92.267	-69.899	13.887
1200	14.000	30.640	21.073	11.480	-92.103	-67.865	12.360
1300	14.240	31.780	21.864	12.891	-91.939	-65.863	11.073
1400	14.470	32.840	22.606	14.327	-91.775	-63.858	9.969
1500	14.710	33.850	23.326	15.786	-91.610	-61.877	9.015
1600	14.940	34.800	24.007	17.269	-91.444	-59.888	8.180
1633	15.019	35.106	24.228	17.763	-91.389	-59.238	7.928
1633	15.019	35.106	24.228	17.763	-92.249	-59.238	7.928
1700	15.180	35.710	24.666	18.775	-92.090	-57.882	7.441
1800	15.410	36.590	25.310	20.304	-91.861	-55.888	6.786
1900	15.640	37.430	25.927	21.856	-91.639	-53.897	6.199
2000	15.870	38.240	26.524	23.432	-91.425	-51.921	5.674

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.340 + 2.280\times10^{-3}T - 1.140\times10^{5}T^{-2}$

$H° - H°_{298} = 11.340\times10^{-3}T + 1.140\times10^{-6}T^{2} + 1.140\times10^{2}T^{-1} - 3.865$

Formation equations (kcal/mol):

298.15-1633 K: $ΔHf° = -94.463 + 2.023\times10^{-3}T - 0.102\times10^{-6}T^{2} + 110.050T^{-1}$

$ΔGf° = -94.463 - 2.023\times10^{-3}T\ln T + 0.102\times10^{-6}T^{2} + 55.025T^{-1} + 36.356\times10^{-3}T$

1633-2000 K: $ΔHf° = -97.712 + 4.272\times10^{-3}T - 0.573\times10^{-6}T^{2} + 64.450T^{-1}$

$ΔGf° = -97.712 - 4.272\times10^{-3}T\ln T + 0.573\times10^{-6}T^{2} + 32.225T^{-1} + 54.223\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (516). Other data from Kubaschewski (289).

$Th_3N_4(c)$

Trithorium Tetranitride

[Formation: $3Th(c) + 2N_2(g) = Th_3N_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	35.200	48.000	48.000	0	-314.300	-289.905	212.504
300	35.280	48.220	48.003	.065	-314.297	-289.755	211.084
400	38.500	58.860	49.428	3.773	-313.978	-281.613	153.864
500	40.320	67.660	52.220	7.720	-313.498	-273.577	119.579
600	41.590	75.130	55.432	11.819	-312.946	-265.644	96.760
700	42.610	81.620	58.720	16.030	-312.370	-257.806	80.490
800	43.490	87.370	61.950	20.336	-311.788	-250.050	68.309
900	44.290	92.540	65.068	24.725	-311.218	-242.371	58.855
1000	45.040	97.240	68.048	29.192	-310.656	-234.746	51.303
1100	45.750	101.570	70.905	33.732	-310.104	-227.183	45.136
1200	46.450	105.580	73.628	38.342	-309.566	-219.670	40.007
1300	47.130	109.330	76.237	43.021	-309.035	-212.201	35.674
1400	47.790	112.840	78.721	47.767	-308.514	-204.763	31.965
1500	48.450	116.160	81.107	52.579	-308.000	-197.375	28.757
1600	49.110	119.310	83.399	57.457	-307.488	-190.019	25.955
1633	49.321	120.315	84.135	59.081	-307.322	-187.598	25.107
1633	49.321	120.315	84.135	59.081	-309.902	-187.598	25.107
1700	49.750	122.310	85.604	62.400	-309.424	-182.595	23.474
1800	50.400	125.170	87.721	67.408	-308.740	-175.153	21.266
1900	51.040	127.910	89.763	72.480	-308.086	-167.744	19.295
2000	51.680	130.550	91.742	77.616	-307.465	-160.389	17.526

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 39.330 + 6.240\text{x}10^{-3}T - 5.330\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 39.330\text{x}10^{-3}T + 3.120\text{x}10^{-6}T^{2} + 5.330\text{x}10^{2}T^{-1} - 13.791$

Formation equations (kcal/mol):

298.15-1633 K: $\Delta Hf° = -318.403 + 8.122\text{x}10^{-3}T - 0.899\text{x}10^{-6}T^{2} + 525.100T^{-1}$

$\Delta Gf° = -318.403 - 8.122\text{x}10^{-3}T\ln T + 0.899\text{x}10^{-6}T^{2} + 262.550T^{-1} + 138.635\text{x}10^{-3}T$

1633-2000 K: $\Delta Hf° = -328.149 + 14.869\text{x}10^{-3}T - 2.312\text{x}10^{-6}T^{2} + 388.300T^{-1}$

$\Delta Gf° = -328.149 - 14.869\text{x}10^{-3}T\ln T + 2.312\text{x}10^{-6}T^{2} + 194.150T^{-1} + 192.237\text{x}10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (516). Other data from Kubaschewski (289).

$ThOBr_2$(c)
Thorium Oxide Dibromide
[Formation: $Th(c) + 0.5O_2(g) + Br_2(l,g) = ThOBr_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	22.340	31.000	31.000	0	-270.000	-257.286	188.594
300	22.368	31.138	31.001	.041	-270.011	-257.207	187.373
332.6	22.754	33.465	31.131	.776	-270.192	-255.807	168.087
332.6	22.754	33.465	31.131	.776	-277.257	-255.807	168.087
400	23.551	37.747	31.895	2.341	-276.973	-251.490	137.406
500	24.255	43.081	33.615	4.733	-276.515	-245.172	107.163
600	24.700	47.550	35.575	7.185	-276.035	-238.947	87.035
700	25.197	51.401	37.567	9.684	-275.546	-232.804	72.684
800	25.576	54.791	39.512	12.223	-275.047	-226.731	61.939
900	25.928	57.824	41.382	14.798	-274.544	-220.724	53.598
1000	26.263	60.573	43.165	17.408	-274.033	-214.771	46.938
1100	26.586	63.091	44.864	20.050	-273.517	-208.868	41.498
1200	26.902	65.418	46.480	22.725	-272.992	-203.014	36.974
1300	27.212	67.584	48.022	25.430	-272.462	-197.205	33.153
1400	27.519	69.612	49.493	28.167	-271.924	-191.435	29.884
1500	27.823	71.520	50.897	30.934	-271.380	-185.706	27.057

*Data estimated.

Phase change: 332.6 K, boiling point of Br_2 ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 23.494 + 2.946 \times 10^{-3}T - 1.806 \times 10^{5}T^{-2}$

$H° - H°_{298} = 23.494 \times 10^{-3}T + 1.473 \times 10^{-6}T^{2} + 1.806 \times 10^{2}T^{-1} - 7.741$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -269.264 - 4.270 \times 10^{-3}T + 0.375 \times 10^{-6}T^{2} + 150.100T^{-1}$

$\Delta Gf° = -269.264 + 4.270 \times 10^{-3}T\ln T - 0.375 \times 10^{-6}T^{2} + 75.050T^{-1} + 15.110 \times 10^{-3}T$

332.6-1500 K: $\Delta Hf° = -279.264 + 4.891 \times 10^{-3}T + 0.220 \times 10^{-6}T^{2} + 118.700T^{-1}$

$\Delta Gf° = -279.264 - 4.891 \times 10^{-3}T\ln T - 0.220 \times 10^{-6}T^{2} + 59.350T^{-1} + 98.465 \times 10^{-3}T$

Source: Data are those estimated by Fuger (163).

$ThOCl_2(c)$
Thorium Oxide Dichloride
[Formation: $Th(c) + 0.5O_2(g) + Cl_2(g) = ThOCl_2(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	21.750	27.400	27.400	0	-294.600	-275.771	202.143
300	21.787	27.535	27.402	.040	-294.594	-275.655	200.812
400	22.068	33.805	28.255	2.220	-294.264	-269.393	147.187
500	23.870	38.944	29.890	4.527	-293.862	-263.218	115.051
600	24.484	43.352	31.775	6.946	-293.396	-257.132	93.659
700	25.009	47.166	33.707	9.421	-292.916	-251.126	78.404
800	25.486	50.537	35.604	11.946	-292.421	-245.189	66.982
900	25.936	53.565	37.435	14.517	-291.915	-239.316	58.113
1000	26.369	56.320	39.188	17.132	-291.392	-233.501	51.031
1100	26.790	58.853	40.862	19.790	-290.854	-227.736	45.246
1200	27.204	61.202	42.460	22.490	-290.303	-222.024	40.436
1300	27.613	63.396	43.988	25.231	-289.734	-216.356	36.372
1400	28.017	65.457	45.448	28.012	-289.150	-210.733	32.897
1500	28.419	67.404	46.848	30.834	-288.549	-205.155	29.891

*Data except enthalpy of formation and entropy at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 21.524 + 4.902\times10^{-3}T - 1.098\times10^{5}T^{-2}$
$H°- H°_{298} = 21.524\times10^{-3}T + 2.451\times10^{-6}T^{2} + 1.098\times10^{2}T^{-1} - 7.004$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = -295.642 + 3.024\times10^{-3}T + 1.165\times10^{-6}T^{2} + 11.000T^{-1}$
$\Delta Gf° = -295.642 - 3.024\times10^{-3}T\ln T - 1.165\times10^{-6}T^{2} + 5.500T^{-1} + 84.162\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation and entropy at 298 K.

$ThOF_2(c)$
Thorium Oxide Difluoride
[Formation: $Th(c) + 0.5O_2(g) + F_2(g) = ThOF_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	20.610	24.200	24.200	0	-399.000	-380.662	279.029
300	20.646	24.328	24.201	.038	-398.995	-380.549	277.226
400	22.022	30.468	25.028	2.176	-398.646	-374.450	204.587
500	22.876	35.478	26.632	4.423	-398.255	-368.446	161.045
600	23.525	39.707	28.469	6.743	-397.849	-362.522	132.047
700	24.077	43.376	30.342	9.124	-397.432	-356.667	111.355
800	24.577	46.624	32.178	11.557	-397.007	-350.873	95.853
900	25.047	49.546	33.948	14.038	-396.570	-345.132	83.809
1000	25.498	52.208	35.642	16.566	-396.121	-339.441	74.184
1100	25.937	54.659	37.262	19.137	-395.660	-333.794	66.318
1200	26.368	56.934	38.806	21.753	-395.183	-328.191	59.771
1300	26.793	59.062	40.284	24.411	-394.689	-322.627	54.238
1400	27.213	61.063	41.698	27.111	-394.182	-317.105	49.502
1500	27.631	62.955	43.053	29.853	-393.659	-311.620	45.402

*Data except enthalpy of formation and entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 21.617 + 4.076\text{x}10^{-3}T - 1.976\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 21.617\text{x}10^{-3}T + 2.038\text{x}10^{-6}T^2 + 1.976\text{x}10^{2}T^{-1} - 7.289$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf^\circ = -400.307 + 3.436\text{x}10^{-3}T + 0.665\text{x}10^{-6}T^2 + 66.600T^{-1}$

$\Delta Gf^\circ = -400.307 - 3.436\text{x}10^{-3}T\ln T - 0.665\text{x}10^{-6}T^2 + 33.300T^{-1} + 85.290\text{x}10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation and entropy at 298 K.

$ThOI_2(c)$
Thorium Oxide Diiodide
[Formation: $Th(c) + 0.5O_2(g) + I_2(c,l,g) = ThOI_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	22.500	34.600	34.600	0	-238.200	-229.130	167.955
300	22.543	34.739	34.600	.042	-238.200	-229.073	166.878
386.8	23.548	40.602	35.312	2.046	-238.288	-226.424	127.932
386.8	23.548	40.602	35.312	2.046	-241.997	-226.424	127.932
400	23.701	41.395	35.500	2.358	-242.076	-225.891	123.419
458.4	24.098	44.654	36.464	3.755	-242.416	-223.503	106.557
458.4	24.098	44.654	36.464	3.755	-252.437	-223.503	106.557
500	24.380	46.760	37.234	4.763	-252.242	-220.884	96.547
600	24.870	51.249	39.204	7.227	-251.759	-214.656	78.188
700	25.272	55.114	41.208	9.734	-251.268	-208.512	65.100
800	25.626	58.512	43.163	12.279	-250.768	-202.437	55.303
900	25.953	61.549	45.040	14.858	-250.268	-196.427	47.698
1000	26.263	64.300	46.831	17.469	-249.760	-190.472	41.627
1100	26.561	66.817	48.534	20.111	-249.249	-184.566	36.669
1200	26.852	69.141	50.157	22.781	-248.735	-178.711	32.547
1300	27.137	71.301	51.700	25.481	-248.214	-172.893	29.066
1400	27.419	73.323	53.174	28.209	-247.691	-167.119	26.088
1500	27.698	75.224	54.581	30.964	-247.164	-161.386	23.514

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 23.762 + 2.684\times10^{-3}T - 1.833\times10^{5}T^{-2}$
$H°-H°_{298} = 23.762\times10^{-3}T + 1.342\times10^{-6}T^2 + 1.833\times10^{2}T^{-1} - 7.819$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -238.954 + 1.212\times10^{-3}T - 1.348\times10^{-6}T^2 + 152.800T^{-1}$
$\Delta Gf° = -238.954 - 1.212\times10^{-3}T\ln T + 1.348\times10^{-6}T^2 + 76.400T^{-1} + 38.593\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -240.409 - 5.192\times10^{-3}T + 0.144\times10^{-6}T^2 + 152.800T^{-1}$
$\Delta Gf° = -240.409 + 5.192\times10^{-3}T\ln T - 0.144\times10^{-6}T^2 + 76.400T^{-1} + 4.778\times10^{-3}T$
458.4-1500 K: $\Delta Hf° = -255.122 + 5.148\times10^{-3}T + 0.076\times10^{-6}T^2 + 137.500T^{-1}$
$\Delta Gf° = -255.122 - 5.148\times10^{-3}T\ln T - 0.076\times10^{-6}T^2 + 68.750T^{-1} + 100.241\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation and entropy at 298 K.

$Th(SO_4)_2(c)$
Thorium Sulfate
[Reaction: $Th(c) + S_2(g) + 4O_2(g) = Th(SO_4)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°$_{298}$)/T	H°- H°$_{298}$	ΔHr°	ΔGr°	
298.15	41.458	40.000	40.000	0	-636.810	-570.237	417.990
300	41.560	40.257	40.000	.077	-636.811	-569.823	415.110
400	47.080	52.969	41.697	4.509	-636.682	-547.503	299.138
500	52.600	64.067	45.081	9.493	-636.136	-525.260	229.588
600	58.120	74.145	49.097	15.029	-635.175	-503.168	183.277
700	63.640	83.519	53.352	21.117	-633.787	-481.271	150.258
800	69.160	92.377	57.681	27.757	-631.956	-459.605	125.557
900	74.680	100.842	62.010	34.949	-629.667	-438.195	106.407
1000	80.200	108.996	66.303	42.693	-626.903	-417.064	91.148

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 25.000 + 55.200 \times 10^{-3}T$

$H° - H°_{298} = 25.000 \times 10^{-3}T + 27.600 \times 10^{-6}T^2 - 9.907$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta Hr° = -632.648 - 18.321 \times 10^{-3}T + 24.321 \times 10^{-6}T^2 - 257.000T^{-1}$

$\Delta Gr° = -632.648 + 18.321 \times 10^{-3}T\ln T - 24.321 \times 10^{-6}T^2 - 128.500T^{-1} + 113.636 \times 10^{-3}T$

Source: Data from Cordfunke (99).

ThSe(g)
Thorium Monoselenide (ideal gas)
[Reaction: Th(c) + $0.5Se_2(g)$ = ThSe(g)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHr°	ΔGr°	
298.15*	8.629	63.180	63.180	0	67.350	60.993	-44.709
300	8.633	63.233	63.180	.016	67.345	60.954	-44.404
400	8.769	65.736	63.521	.886	67.053	58.867	-32.163
500	8.888	67.704	64.168	1.768	66.743	56.855	-24.851
600	9.086	69.340	64.897	2.666	66.429	54.907	-20.000
700	9.412	70.764	65.635	3.590	66.121	53.012	-16.551
800	9.854	72.049	66.358	4.553	65.834	51.162	-13.977
900	10.363	73.239	67.057	5.564	65.576	49.342	-11.982
1000	10.873	74.357	67.731	6.626	65.354	47.549	-10.392
1100	11.328	75.416	68.382	7.737	65.163	45.780	-9.096
1200	11.696	76.418	69.010	8.889	64.997	44.025	-8.018
1300	11.944	77.365	69.617	10.072	64.847	42.287	-7.109
1400	12.090	78.256	70.203	11.274	64.700	40.554	-6.331
1500	12.142	79.092	70.768	12.486	64.546	38.833	-5.658
1600	12.118	79.875	71.313	13.700	64.380	37.124	-5.071
1633	12.091	80.122	71.488	14.099	64.319	36.562	-4.893
1633	12.091	80.122	71.488	14.099	63.459	36.562	-4.893
1700	12.037	80.608	71.839	14.908	63.377	35.466	-4.559
1800	11.916	81.292	72.344	16.106	63.222	33.825	-4.107
1900	11.770	81.933	72.833	17.290	63.029	32.194	-3.703
2000	11.610	82.532	73.302	18.459	62.795	30.575	-3.341

*Data estimated.

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.864 + 2.670\times10^{-3}T - 0.028\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.864\times10^{-3}T + 1.335\times10^{-6}T^{2} + 0.028\times10^{2}T^{-1} - 2.473$

Reaction equations (kcal/mol):

298.15-1633 K: $\Delta Hr^\circ = 68.470 - 3.526\times10^{-3}T + 0.548\times10^{-6}T^{2} - 35.050T^{-1}$

$\Delta Gr^\circ = 68.470 + 3.526\times10^{-3}T\ln T - 0.548\times10^{-6}T^{2} - 17.525T^{-1} - 44.806\times10^{-3}T$

1633-2000 K: $\Delta Hr^\circ = 65.221 - 1.277\times10^{-3}T + 0.077\times10^{-6}T^{2} - 80.650T^{-1}$

$\Delta Gr^\circ = 65.221 + 1.277\times10^{-3}T\ln T - 0.077\times10^{-6}T^{2} - 40.325T^{-1} - 26.939\times10^{-3}T$

Source: Data are those estimated by Gronvold (187).

$ThSe_2(g)$
Thorium Diselenide (ideal gas)
[Reaction: $Th(c) + Se_2(g) = ThSe_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	13.243	78.070	78.070	0	12.700	10.580	-7.755
300	13.250	78.152	78.070	.025	12.695	10.567	-7.698
400	13.524	82.005	78.595	1.364	12.374	9.905	-5.412
500	13.659	85.038	79.590	2.724	12.039	9.326	-4.077
600	13.734	87.535	80.712	4.094	11.691	8.815	-3.211
700	13.780	89.656	81.842	5.470	11.330	8.366	-2.612
800	13.810	91.498	82.937	6.849	10.955	7.972	-2.178
900	13.831	93.126	83.980	8.231	10.566	7.619	-1.850
1000	13.846	94.584	84.969	9.615	10.166	7.310	-1.598
1100	13.857	95.904	85.904	11.000	9.753	7.048	-1.400
1200	13.865	97.110	86.787	12.387	9.328	6.821	-1.242
1300	13.872	98.221	87.626	13.773	8.889	6.633	-1.115
1400	13.877	99.249	88.420	15.161	8.439	6.472	-1.010
1500	13.882	100.206	89.173	16.549	7.976	6.347	-.925
1600	13.885	101.102	89.891	17.937	7.501	6.250	-.854
1633	13.886	101.385	90.121	18.395	7.341	6.225	-.833
1633	13.886	101.385	90.121	18.395	6.481	6.225	-.833
1700	13.888	101.944	90.576	19.326	6.200	6.236	-.802
1800	13.890	102.738	91.230	20.715	5.760	6.241	-.758
1900	13.892	103.489	91.855	22.104	5.298	6.277	-.722
2000	13.894	104.202	92.456	23.493	4.814	6.334	-.692

*Data estimated.

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.872 + 0.026\times10^{-3}T - 0.566\times10^{5}T^{-2}$

$H° - H°_{298} = 13.872\times10^{-3}T + 0.013\times10^{-6}T^{2} + 0.566\times10^{2}T^{-1} - 4.327$

Reaction equations (kcal/mol):

298.15-1633 K: $\Delta Hr° = 13.642 - 2.850\times10^{-3}T - 0.615\times10^{-6}T^{2} - 11.200T^{-1}$

$\Delta Gr° = 13.642 + 2.850\times10^{-3}T\ln T + 0.615\times10^{-6}T^{2} - 5.600T^{-1} - 26.628\times10^{-3}T$

1633-2000 K: $\Delta Hr° = 10.393 - 0.601\times10^{-3}T - 1.086\times10^{-6}T^{2} - 56.800T^{-1}$

$\Delta Gr° = 10.393 + 0.601\times10^{-3}T\ln T + 1.086\times10^{-6}T^{2} - 28.400T^{-1} - 8.761\times10^{-3}T$

Source: Data are those estimated by Gronvold (187).

ThTe(g)
Thorium Monotelluride (ideal gas)
[Reaction: $Th(c) + 0.5Te_2(g) = ThTe(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°$_{298}$)/T	H°- H°$_{298}$	ΔHr°	ΔGr°	
298.15*	8.761	65.090	65.090	0	77.835	71.456	-52.378
300	8.763	65.144	65.091	.016	77.831	71.416	-52.026
400	8.888	67.680	65.435	.898	77.609	69.311	-37.869
500	9.119	69.684	66.090	1.797	77.372	67.264	-29.401
600	9.538	71.382	66.835	2.728	77.140	65.266	-23.773
700	10.112	72.894	67.594	3.710	76.930	63.304	-19.764
800	10.736	74.286	68.345	4.753	76.755	61.369	-16.765
900	11.303	75.585	69.078	5.856	76.610	59.452	-14.437
1000	11.737	76.799	69.789	7.010	76.490	57.554	-12.578
1100	12.011	77.932	70.479	8.198	76.377	55.668	-11.060
1200	12.133	78.983	71.145	9.406	76.257	53.790	-9.796
1300	12.131	79.955	71.786	10.620	76.116	51.924	-8.729
1400	12.039	80.851	72.402	11.829	75.944	50.069	-7.816
1500	11.888	81.677	72.993	13.026	75.738	48.225	-7.026
1600	11.704	82.438	73.559	14.206	75.498	46.397	-6.337
1633	11.639	82.676	73.741	14.591	75.410	45.798	-6.129
1633	11.639	82.676	73.741	14.591	74.550	45.798	-6.129
1700	11.506	83.142	74.103	15.366	74.406	44.627	-5.737
1800	11.306	83.794	74.623	16.507	74.152	42.878	-5.206
1900	11.112	84.400	75.122	17.628	73.851	41.150	-4.733
2000	10.929	84.965	75.600	18.730	73.505	39.439	-4.310

*Data estimated.

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.380 + 1.636x10^{-3}T - 0.984x10^{5}T^{-2}$
$H° - H°_{298} = 9.380x10^{-3}T + 0.818x10^{-6}T^{2} + 0.984x10^{2}T^{-1} - 3.199$

Reaction equations (kcal/mol):

298.15-1633 K: $\Delta Hr° = 77.901 - 0.978x10^{-3}T - 0.426x10^{-6}T^{2} + 78.400T^{-1}$
$\Delta Gr° = 77.901 + 0.978x10^{-3}T\ln T + 0.426x10^{-6}T^{2} + 39.200T^{-1} - 27.755x10^{-3}T$
1633-2000 K: $\Delta Hr° = 74.653 + 1.271x10^{-3}T - 0.897x10^{-6}T^{2} + 32.800T^{-1}$
$\Delta Gr° = 74.653 - 1.271x10^{-3}T\ln T + 0.897x10^{-6}T^{2} + 16.400T^{-1} - 9.887x10^{-3}T$

Source: Data are those estimated by Gronvold (187).

$ThTe_2(g)$
Thorium Ditelluride (ideal gas)
[Reaction: $Th(c) + Te_2(g) = ThTe_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	13.472	81.600	81.600	0	30.670	28.592	-20.958
300	13.477	81.683	81.600	.025	30.667	28.578	-20.819
400	13.661	85.588	82.131	1.383	30.481	27.911	-15.249
500	13.749	88.646	83.140	2.753	30.268	27.291	-11.929
600	13.797	91.158	84.273	4.131	30.026	26.722	-9.734
700	13.827	93.287	85.413	5.512	29.751	26.192	-8.177
800	13.846	95.135	86.515	6.896	29.443	25.702	-7.021
900	13.860	96.766	87.565	8.281	29.100	25.253	-6.132
1000	13.869	98.227	88.559	9.668	28.724	24.845	-5.430
1100	13.876	99.549	89.499	11.055	28.314	24.482	-4.864
1200	13.862	100.757	90.388	12.443	27.868	24.153	-4.399
1300	13.886	101.868	91.229	13.831	27.389	23.863	-4.012
1400	13.889	102.897	92.026	15.220	26.876	23.610	-3.686
1500	13.892	103.856	92.783	16.609	26.340	23.391	-3.408
1600	13.894	104.752	93.503	17.998	25.787	23.208	-3.170
1633	13.895	105.036	93.733	18.457	25.600	23.156	-3.099
1633	13.895	105.036	93.733	18.457	24.740	23.156	-3.099
1700	13.896	105.595	94.190	19.388	24.404	23.112	-2.971
1800	13.898	106.389	94.846	20.778	23.879	23.044	-2.798
1900	13.899	107.141	95.474	22.167	23.329	23.012	-2.647
2000	13.900	107.853	96.075	23.557	22.756	23.014	-2.515

*Data estimated.

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.892 + 0.012\times10^{-3}T - 0.377\times10^{5}T^{-2}$

$H°-H°_{298} = 13.892\times10^{-3}T + 0.006\times10^{-6}T^{2} + 0.377\times10^{2}T^{-1} - 4.269$

Reaction equations (kcal/mol):

298.15-1633 K: $\Delta Hr° = 31.016 - 0.765\times10^{-3}T - 1.534\times10^{-6}T^{2} + 5.600T^{-1}$

$\Delta Gr° = 31.016 + 0.765\times10^{-3}T\ln T + 1.534\times10^{-6}T^{2} + 2.800T^{-1} - 12.977\times10^{-3}T$

1633-2000 K: $\Delta Hr° = 27.767 + 1.484\times10^{-3}T - 2.005\times10^{-6}T^{2} - 40.000T^{-1}$

$\Delta Gr° = 27.767 - 1.484\times10^{-3}T\ln T + 2.005\times10^{-6}T^{2} - 20.000T^{-1} + 4.890\times10^{-3}T$

Source: Data are those estimated by Gronvold (187).

$TiAl_3(c)$
Titanium Aluminide
[Formation: $Ti(c) + 3Al(c,l) = TiAl_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	21.630	22.080	22.080	0	-35.000	-33.340	24.438
300	21.670	22.210	22.080	.040	-35.004	-33.328	24.279
400	23.110	28.670	22.952	2.287	-35.167	-32.747	17.892
500	23.970	33.920	24.632	4.644	-35.325	-32.122	14.040
600	24.570	38.350	26.562	7.073	-35.513	-31.463	11.460
700	25.040	42.170	28.521	9.554	-35.767	-30.760	9.604
800	25.460	45.540	30.441	12.079	-36.112	-30.024	8.202
900	25.870	48.570	32.298	14.645	-36.564	-29.245	7.102
933.61	26.018	49.521	32.901	15.517	-36.740	-28.968	6.781
933.61	26.018	49.521	32.901	15.517	-44.480	-28.968	6.781
1000	26.310	51.310	34.057	17.253	-44.764	-27.847	6.086
1100	26.810	53.840	35.741	19.909	-45.168	-26.142	5.194
1156	27.146	55.181	36.653	21.419	-45.381	-25.166	4.758
1156	27.146	55.181	36.653	21.419	-46.398	-25.166	4.758
1200	27.410	56.200	37.351	22.619	-46.510	-24.356	4.436
1300	28.140	58.420	38.885	25.396	-46.731	-22.499	3.782
1400	29.040	60.540	40.359	28.253	-46.892	-20.631	3.221

Phase changes: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp° = 22.899 + 3.752\times10^{-3}T - 2.122\times10^{5}T^{-2}$

$H° - H°_{298} = 22.899\times10^{-3}T + 1.876\times10^{-6}T^{2} + 2.122\times10^{2}T^{-1} - 7.706$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -36.531 + 3.646\times10^{-3}T - 4.428\times10^{-6}T^{2} + 249.600T^{-1}$

$\Delta Gf° = -36.531 - 3.646\times10^{-3}T\ln T + 4.428\times10^{-6}T^{2} + 124.800T^{-1} + 28.751\times10^{-3}T$

933.61-1156 K: $\Delta Hf° = -40.334 - 5.348\times10^{-3}T + 0.753\times10^{-6}T^{2} + 197.400T^{-1}$

$\Delta Gf° = -40.334 + 5.348\times10^{-3}T\ln T - 0.753\times10^{-6}T^{2} + 98.700T^{-1} - 23.819\times10^{-3}T$

1156-1400 K: $\Delta Hf° = -44.371 - 2.948\times10^{-3}T + 0.430\times10^{-6}T^{2} + 980.300T^{-1}$

$\Delta Gf° = -44.371 + 2.948\times10^{-3}T\ln T - 0.430\times10^{-6}T^{2} + 490.150T^{-1} - 4.067\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Other data from Stuve (481).

TiB(c)
Titanium Boride
[Formation: Ti(c,l) + B(β) = TiB(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.092	8.300	8.300	0	-38.300	-38.172	27.980
300	7.150	8.344	8.301	.013	-38.303	-38.169	27.806
400	9.640	10.771	8.613	.863	-38.386	-38.110	20.822
500	10.926	13.071	9.279	1.896	-38.403	-38.038	16.626
600	11.608	15.128	10.086	3.025	-38.413	-37.968	13.830
700	11.980	16.948	10.939	4.206	-38.439	-37.885	11.828
800	12.168	18.560	11.792	5.414	-38.490	-37.802	10.327
900	12.306	20.002	12.626	6.638	-38.573	-37.711	9.157
1000	12.408	21.304	13.430	7.874	-38.683	-37.607	8.219
1100	12.474	22.490	14.201	9.118	-38.826	-37.506	7.452
1156	12.492	23.110	14.618	9.817	-38.920	-37.432	7.077
1156	12.492	23.110	14.618	9.817	-39.937	-37.432	7.077
1200	12.506	23.577	14.938	10.367	-39.971	-37.336	6.800
1300	12.538	24.579	15.641	11.620	-40.073	-37.108	6.238
1400	12.570	25.509	16.313	12.875	-40.207	-36.875	5.756
1500	12.602	26.378	16.955	14.134	-40.371	-36.627	5.336
1600	12.634	27.192	17.570	15.395	-40.570	-36.384	4.970
1700	12.666	27.959	18.159	16.660	-40.803	-36.114	4.643
1800	12.698	28.684	18.723	17.929	-41.076	-35.820	4.349
1900	12.730	29.371	19.266	19.200	-41.397	-35.517	4.085
1945	12.744	29.669	19.503	19.773	-41.559	-35.377	3.975
1945	12.744	29.669	19.503	19.773	-44.859	-35.377	3.975
2000	12.762	30.025	19.788	20.475	-45.171	-35.117	3.837

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.049 - 0.122\times10^{-3}T - 5.263\times10^{5}T^{-2}$
$H°- H°_{298} = 13.049\times10^{-3}T - 0.061\times10^{-6}T^{2} + 5.263\times10^{2}T^{-1} - 5.650$

Formation equations (kcal/mol):

298.15-1156 K: $ΔHf° = -39.955 + 2.849\times10^{-3}T - 1.876\times10^{-6}T^{2} + 290.000T^{-1}$
$ΔGf° = -39.955 - 2.849\times10^{-3}T\ln T + 1.876\times10^{-6}T^{2} + 145.000T^{-1} + 20.024\times10^{-3}T$
1156-1945 K: $ΔHf° = -43.992 + 5.249\times10^{-3}T - 2.199\times10^{-6}T^{2} + 1072.900T^{-1}$
$ΔGf° = -43.992 - 5.249\times10^{-3}T\ln T + 2.199\times10^{-6}T^{2} + 536.450T^{-1} + 39.776\times10^{-3}T$
1945-2000 K: $ΔHf° = -36.860 - 2.724\times10^{-3}T - 0.753\times10^{-6}T^{2} + 304.800T^{-1}$
$ΔGf° = -36.860 + 2.724\times10^{-3}T\ln T + 0.753\times10^{-6}T^{2} + 152.400T^{-1} - 21.356\times10^{-3}T$

Source: Data from JANAF (127) who estimated all except enthalpy of formation at 298 K.

$TiB_2(c)$
Titanium Diboride
[Formation: $Ti(c,l) + 2B(\beta) = TiB_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	10.583	6.808	6.808	0	-78.500	-77.507	56.813
300	10.641	6.874	6.808	.020	-78.501	-77.497	56.456
400	13.119	10.310	7.260	1.220	-78.551	-77.159	42.157
500	14.739	13.422	8.186	2.618	-78.610	-76.801	33.569
600	15.814	16.208	9.296	4.147	-78.695	-76.438	27.842
700	16.610	18.708	10.465	5.770	-78.797	-76.045	23.742
800	17.225	20.966	11.638	7.462	-78.910	-75.643	20.664
900	17.814	23.029	12.791	9.214	-79.034	-75.226	18.267
1000	18.377	24.936	13.912	11.024	-79.158	-74.794	16.346
1100	18.914	26.713	14.996	12.889	-79.284	-74.370	14.776
1156	19.201	27.659	15.586	13.956	-79.355	-74.111	14.011
1156	19.201	27.659	15.586	13.956	-80.372	-74.111	14.011
1200	19.427	28.380	16.042	14.806	-80.380	-73.872	13.454
1300	19.914	29.955	17.053	16.773	-80.402	-73.323	12.327
1400	20.375	31.448	18.028	18.788	-80.424	-72.779	11.361
1500	20.810	32.868	18.969	20.848	-80.450	-72.221	10.522
1600	21.219	34.225	19.882	22.949	-80.487	-71.698	9.793
1700	21.602	35.523	20.764	25.090	-80.536	-71.145	9.146
1800	21.959	36.768	21.619	27.269	-80.605	-70.568	8.568
1900	22.290	37.964	22.448	29.481	-80.705	-70.004	8.052
1945	22.427	38.487	22.813	30.487	-80.763	-69.751	7.837
1945	22.427	38.487	22.813	30.487	-84.063	-69.751	7.837
2000	22.595	39.115	23.252	31.726	-84.243	-69.369	7.580

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H^\circ = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H^\circ = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.310 + 4.466\times10^{-3}T - 4.496\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 14.310\times10^{-3}T + 2.233\times10^{-6}T^2 + 4.496\times10^{2}T^{-1} - 5.973$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf^\circ = -78.265 - 0.613\times10^{-3}T - 0.274\times10^{-6}T^2 - 8.200T^{-1}$
$\Delta Gf^\circ = -78.265 + 0.613\times10^{-3}T\ln T + 0.274\times10^{-6}T^2 - 4.100T^{-1} - 0.983\times10^{-3}T$
1156-1945 K: $\Delta Hf^\circ = -82.302 + 1.787\times10^{-3}T - 0.597\times10^{-6}T^2 + 774.700T^{-1}$
$\Delta Gf^\circ = -82.302 - 1.787\times10^{-3}T\ln T + 0.597\times10^{-6}T^2 + 387.350T^{-1} + 18.769\times10^{-3}T$
1945-2000 K: $\Delta Hf^\circ = -75.170 - 6.186\times10^{-3}T + 0.849\times10^{-6}T^2 + 6.600T^{-1}$
$\Delta Gf^\circ = -75.170 + 6.186\times10^{-3}T\ln T - 0.849\times10^{-6}T^2 + 3.300T^{-1} - 42.363\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Topor (500). Other data from JANAF (127).

TiC(c)
Titanium Carbide
[Formation: Ti(c,l) + C(c) = TiC(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.070	5.790	5.790	0	-44.100	-43.235	31.692
300	8.109	5.840	5.790	.015	-44.100	-43.228	31.492
400	9.663	8.406	6.129	.911	-44.064	-42.941	23.462
500	10.593	10.670	6.816	1.927	-44.008	-42.669	18.651
600	11.192	12.659	7.629	3.018	-43.958	-42.407	15.447
700	11.588	14.416	8.475	4.159	-43.930	-42.145	13.158
800	11.855	15.981	9.316	5.332	-43.929	-41.891	11.444
900	12.044	17.389	10.137	6.527	-43.959	-41.635	10.110
1000	12.188	18.666	10.927	7.739	-44.012	-41.373	9.042
1100	12.312	19.833	11.684	8.964	-44.094	-41.101	8.166
1156	12.380	20.447	12.094	9.655	-44.151	-40.955	7.743
1156	12.380	20.447	12.094	9.655	-45.168	-40.955	7.743
1200	12.434	20.910	12.409	10.201	-45.170	-40.795	7.430
1300	12.567	21.910	13.102	11.451	-45.191	-40.429	6.797
1400	12.718	22.847	13.765	12.715	-45.227	-40.062	6.254
1500	12.890	23.730	14.399	13.996	-45.274	-39.689	5.783
1600	13.084	24.568	15.009	15.294	-45.332	-39.316	5.370
1700	13.300	25.368	15.596	16.613	-45.401	-38.939	5.006
1800	13.534	26.135	16.160	17.955	-45.482	-38.557	4.681
1900	13.784	26.873	16.705	19.320	-45.581	-38.169	4.390
1945	13.902	27.197	16.944	19.943	-45.633	-37.994	4.269
1945	13.902	27.197	16.944	19.943	-48.933	-37.994	4.269
2000	14.046	27.587	17.231	20.712	-49.102	-37.682	4.118
2100	14.318	28.278	17.740	22.130	-49.391	-37.104	3.861
2200	14.598	28.951	18.235	23.576	-49.656	-36.513	3.627
2300	14.887	29.606	18.715	25.050	-49.897	-35.906	3.412
2400	15.190	30.246	19.182	26.554	-50.113	-35.295	3.214
2500	15.512	30.873	19.638	28.088	-50.301	-34.676	3.031
2600	15.865	31.488	20.081	29.657	-50.459	-34.048	2.862
2700	16.265	32.094	20.515	31.263	-50.583	-33.414	2.705
2800	16.733	32.694	20.940	32.912	-50.667	-32.778	2.558

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2800 K: $C_p^\circ = 10.674 + 1.774\times10^{-3}T - 2.785\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.674\times10^{-3}T + 0.887\times10^{-6}T^{2} + 2.785\times10^{2}T^{-1} - 4.195$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf^\circ = -44.818 + 1.679\times10^{-3}T - 1.002\times10^{-6}T^{2} + 91.400T^{-1}$
$\Delta Gf^\circ = -44.818 - 1.679\times10^{-3}T\ln T + 1.002\times10^{-6}T^{2} + 45.700T^{-1} + 14.064\times10^{-3}T$
1156-1945 K: $\Delta Hf^\circ = -48.855 + 4.079\times10^{-3}T - 1.325\times10^{-6}T^{2} + 874.300T^{-1}$
$\Delta Gf^\circ = -48.855 - 4.079\times10^{-3}T\ln T + 1.325\times10^{-6}T^{2} + 437.150T^{-1} + 33.816\times10^{-3}T$
1945-2000 K: $\Delta Hf^\circ = -41.723 - 3.894\times10^{-3}T + 0.121\times10^{-6}T^{2} + 106.200T^{-1}$
$\Delta Gf^\circ = -41.723 + 3.894\times10^{-3}T\ln T - 0.121\times10^{-6}T^{2} + 53.100T^{-1} - 27.316\times10^{-3}T$
2000-2800 K: $\Delta Hf^\circ = -39.731 - 6.017\times10^{-3}T + 0.753\times10^{-6}T^{2} - 441.500T^{-1}$
$\Delta Gf^\circ = -39.731 + 6.017\times10^{-3}T\ln T - 0.753\times10^{-6}T^{2} - 220.750T^{-1} - 43.116\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Low-temperature heat capacities and entropy at 298 K from Kelley (242). High-temperature data based on Naylor (352), Turchanin (505), and Levinson (302).

$TiH_2(c)$
Titanium Dihydride
[Formation: $Ti(c,l) + H_2(g) = TiH_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.191	7.101	7.101	0	-28.600	-19.230	14.096
300	7.232	7.146	7.103	.013	-28.611	-19.172	13.966
400*	9.400	9.524	7.412	.845	-29.089	-15.948	8.713
500	11.300	11.832	8.066	1.883	-29.393	-12.626	5.519
600	12.860	14.035	8.878	3.094	-29.546	-9.256	3.371
700	14.100	16.115	9.765	4.445	-29.586	-5.864	1.831
800	15.090	18.065	10.683	5.906	-29.544	-2.478	.677
900	15.850	19.888	11.605	7.455	-29.444	.900	-.219
1000	16.380	21.588	12.520	9.068	-29.307	4.265	-.932
1100	16.744	23.166	13.416	10.725	-29.159	7.610	-1.512
1156	16.915	24.003	13.909	11.668	-29.075	9.483	-1.793
1156	16.915	24.003	13.909	11.668	-30.092	9.483	-1.793
1200	17.050	24.637	14.291	12.415	-29.980	10.987	-2.001
1300	17.298	26.012	15.140	14.133	-29.729	14.390	-2.419
1400	17.488	27.301	15.963	15.873	-29.486	17.775	-2.775
1500	17.620	28.512	16.759	17.629	-29.257	21.145	-3.081
1600	17.753	29.654	17.530	19.398	-29.047	24.495	-3.346
1700	17.858	30.734	18.276	21.178	-28.860	27.837	-3.579
1800	17.934	31.757	18.997	22.968	-28.703	31.165	-3.784
1900	17.981	32.728	19.694	24.764	-28.585	34.489	-3.967
1945	17.990	33.149	20.001	25.573	-28.548	35.982	-4.043
1945	17.990	33.149	20.001	25.573	-31.848	35.982	-4.043
2000	18.000	33.650	20.368	26.564	-31.915	37.903	-4.142

*Data above 363 K estimated.

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.266 + 3.870\times10^{-3}T - 5.537\times10^{5}T^{-2}$
$H°- H°_{298} = 12.266\times10^{-3}T + 1.935\times10^{-6}T^{2} + 5.537\times10^{2}T^{-1} - 5.686$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -30.597 + 0.333\times10^{-3}T + 0.393\times10^{-6}T^{2} + 555.400T^{-1}$
$\Delta Gf° = -30.597 - 0.333\times10^{-3}T\ln T - 0.393\times10^{-6}T^{2} + 277.700T^{-1} + 37.015\times10^{-3}T$
1156-1945 K: $\Delta Hf° = -34.634 + 2.733\times10^{-3}T + 0.070\times10^{-6}T^{2} + 1338.300T^{-1}$
$\Delta Gf° = -34.634 - 2.733\times10^{-3}T\ln T - 0.070\times10^{-6}T^{2} + 669.150T^{-1} + 56.767\times10^{-3}T$
1945-2000 K: $\Delta Hf° = -27.502 - 5.240\times10^{-3}T + 1.516\times10^{-6}T^{2} + 570.200T^{-1}$
$\Delta Gf° = -27.502 + 5.240\times10^{-3}T\ln T - 1.516\times10^{-6}T^{2} + 285.100T^{-1} - 4.366\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Other data from JANAF (127) who estimated all above 363 K.

TiN(c)
Titanium Nitride
[Formation: $Ti(c,l) + 0.5N_2(g) = TiN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.860	7.230	7.230	0	-80.800	-73.950	54.206
300	8.901	7.285	7.232	.016	-80.802	-73.907	53.841
400	10.379	10.074	7.599	.990	-80.792	-71.606	39.123
500	11.132	12.479	8.341	2.069	-80.708	-69.321	30.300
600	11.596	14.552	9.207	3.207	-80.590	-67.054	24.424
700	11.923	16.366	10.105	4.383	-80.466	-64.803	20.232
800	12.177	17.975	10.989	5.589	-80.345	-62.574	17.094
900	12.388	19.422	11.848	6.817	-80.235	-60.359	14.657
1000	12.573	20.737	12.672	8.065	-80.132	-58.155	12.710
1100	12.742	21.943	13.460	9.331	-80.043	-55.968	11.120
1156	12.829	22.578	13.887	10.047	-79.998	-54.741	10.349
1156	12.829	22.578	13.887	10.047	-81.015	-54.741	10.349
1200	12.898	23.059	14.215	10.613	-80.936	-53.742	9.788
1300	13.046	24.097	14.935	11.911	-80.765	-51.481	8.655
1400	13.188	25.069	15.625	13.222	-80.605	-49.236	7.686
1500	13.326	25.983	16.284	14.548	-80.454	-46.998	6.848
1600	13.460	26.848	16.919	15.887	-80.315	-44.775	6.116
1700	13.592	27.668	17.527	17.240	-80.189	-42.557	5.471
1800	13.721	28.448	18.111	18.606	-80.083	-40.346	4.899
1900	13.849	29.194	18.676	19.984	-80.004	-38.142	4.387
1945	13.906	29.519	18.923	20.608	-79.979	-37.152	4.175
1945	13.906	29.519	18.923	20.608	-83.279	-37.152	4.175
2000	13.976	29.907	19.219	21.376	-83.356	-35.845	3.917

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.663 + 1.192\text{x}10^{-3}T - 2.820\text{x}10^{5}T^{-2}$
$H°- H^\circ_{298} = 11.663\text{x}10^{-3}T + 0.596\text{x}10^{-6}T^{2} + 2.820\text{x}10^{2}T^{-1} - 4.476$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -82.509 + 2.927\text{x}10^{-3}T - 0.822\text{x}10^{-6}T^{2} + 271.150T^{-1}$
$\Delta Gf° = -82.509 - 2.927\text{x}10^{-3}T\ln T + 0.822\text{x}10^{-6}T^{2} + 135.575T^{-1} + 43.617\text{x}10^{-3}T$
1156-1945 K: $\Delta Hf° = -86.546 + 5.327\text{x}10^{-3}T - 1.145\text{x}10^{-6}T^{2} + 1054.050T^{-1}$
$\Delta Gf° = -86.546 - 5.327\text{x}10^{-3}T\ln T + 1.145\text{x}10^{-6}T^{2} + 527.025T^{-1} + 63.370\text{x}10^{-3}T$
1945-2000 K: $\Delta Hf° = -79.414 - 2.645\text{x}10^{-3}T + 0.301\text{x}10^{-6}T^{2} + 285.950T^{-1}$
$\Delta Gf° = -79.414 + 2.645\text{x}10^{-3}T\ln T - 0.301\text{x}10^{-6}T^{2} + 142.975T^{-1} + 2.237\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Low-temperature heat capacities and entropy at 298 K from Shomate (451). High-temperature data based on Naylor (352).

TiO(α)
α-Titanium Monoxide
[Formation: Ti(c) + 0.5O$_2$(g) = TiO(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H$^\circ_{298}$)/T	H°- H$^\circ_{298}$	ΔHf°	ΔGf°	
298.15	9.560	8.190	8.190	0	-129.700	-122.654	89.907
300	9.570	8.250	8.190	.018	-129.699	-122.609	89.320
400	10.830	11.200	8.585	1.046	-129.642	-120.252	65.702
500	11.530	13.700	9.366	2.167	-129.530	-117.920	51.542
600	12.050	15.850	10.253	3.358	-129.380	-115.599	42.107
700	12.480	17.740	11.207	4.573	-129.243	-113.320	35.380
800	12.900	19.430	12.128	5.842	-129.086	-111.054	30.338
900	13.300	20.970	13.023	7.152	-128.921	-108.807	26.422
1000	13.720	22.400	13.897	8.503	-128.742	-106.587	23.294
1100	14.140	23.720	14.724	9.896	-128.551	-104.379	20.738
1156	14.392	24.429	15.177	10.694	-128.438	-103.149	19.501
1156	14.392	24.429	15.177	10.694	-129.455	-103.149	19.501
1200	14.590	24.970	15.527	11.332	-129.314	-102.150	18.604
1265	14.890	25.750	16.035	12.290	-129.101	-100.688	17.395

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1265 K, α - β transition point of TiO: ΔH° = 1.290 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1265 K: $Cp^\circ = 10.457 + 3.466\text{x}10^{-3}T - 1.716\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.457\text{x}10^{-3}T + 1.733\text{x}10^{-6}T^{2} + 1.716\text{x}10^{2}T^{-1} - 3.847$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf^\circ = -130.589 + 1.365\text{x}10^{-3}T + 0.359\text{x}10^{-6}T^{2} + 134.200T^{-1}$
$\Delta Gf^\circ = -130.589 - 1.365\text{x}10^{-3}T\ln T - 0.359\text{x}10^{-6}T^{2} + 67.100T^{-1} + 33.743\text{x}10^{-3}T$
1156-1265 K: $\Delta Hf^\circ = -134.626 + 3.765\text{x}10^{-3}T + 0.036\text{x}10^{-6}T^{2} + 917.100T^{-1}$
$\Delta Gf^\circ = -134.626 - 3.765\text{x}10^{-3}T\ln T - 0.036\text{x}10^{-6}T^{2} + 458.550T^{-1} + 53.496\text{x}10^{-3}T$

Source: Data from Beyer (40).

$TiOCl(g)$
Titanium Oxychloride (ideal gas)
[Formation: $Ti(c,l) + 0.5Cl_2(g) + 0.5O_2(g) = TiOCl(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	12.346	62.992	62.992	0	-58.400	-59.749	43.797
300	12.365	63.069	62.992	.023	-58.402	-59.756	43.532
400	13.170	66.745	63.488	1.303	-58.508	-60.191	32.886
500	13.671	69.742	64.448	2.647	-58.599	-60.603	26.489
600	13.993	72.266	65.548	4.031	-58.691	-60.996	22.217
700	14.208	74.440	66.666	5.442	-58.797	-61.365	19.159
800	14.357	76.347	67.758	6.871	-58.923	-61.725	16.862
900	14.464	78.045	68.809	8.312	-59.072	-62.066	15.072
1000	14.543	79.573	69.811	9.762	-59.241	-62.390	13.635
1100	14.602	80.962	70.762	11.220	-59.434	-62.701	12.457
1156	14.628	81.688	71.275	12.038	-59.552	-62.862	11.884
1156	14.628	81.688	71.275	12.038	-60.569	-62.862	11.884
1200	14.649	82.235	71.667	12.682	-60.621	-62.949	11.464
1300	14.685	83.409	72.525	14.149	-60.754	-63.137	10.614
1400	14.714	84.498	73.342	15.619	-60.909	-63.314	9.884
1500	14.738	85.514	74.119	17.092	-61.084	-63.479	9.249
1600	14.758	86.466	74.862	18.567	-61.283	-63.633	8.692
1700	14.774	87.361	75.571	20.043	-61.509	-63.772	8.198
1800	14.788	88.206	76.249	21.522	-61.765	-63.899	7.758
1900	14.800	89.006	76.900	23.001	-62.061	-64.008	7.363
1945	14.805	89.352	77.184	23.667	-62.209	-64.054	7.197
1945	14.805	89.352	77.184	23.667	-65.509	-64.054	7.197
2000	14.810	89.765	77.524	24.481	-65.803	-64.009	6.994

*Data estimated.

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.146 + 0.494\times10^{-3}T - 1.731\times10^{5}T^{-2}$
$H°- H°_{298} = 14.146\times10^{-3}T + 0.247\times10^{-6}T^{2} + 1.731\times10^{2}T^{-1} - 4.820$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -58.827 + 0.640\times10^{-3}T - 1.171\times10^{-6}T^{2} + 101.550T^{-1}$
$\Delta Gf° = -58.827 - 0.640\times10^{-3}T\ln T + 1.171\times10^{-6}T^{2} + 50.775T^{-1} - 0.362\times10^{-3}T$
1156-1945 K: $\Delta Hf° = -62.864 + 3.040\times10^{-3}T - 1.494\times10^{-6}T^{2} + 884.450T^{-1}$
$\Delta Gf° = -62.864 - 3.040\times10^{-3}T\ln T + 1.494\times10^{-6}T^{2} + 442.225T^{-1} + 19.390\times10^{-3}T$
1945-2000 K: $\Delta Hf° = -55.732 - 4.933\times10^{-3}T - 0.048\times10^{-6}T^{2} + 116.350T^{-1}$
$\Delta Gf° = -55.732 + 4.933\times10^{-3}T\ln T + 0.048\times10^{-6}T^{2} + 58.175T^{-1} - 41.742\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$TiOCl_2(g)$
Titanium Oxide Dichloride (ideal gas)
[Formation: $Ti(c,l) + Cl_2(g) + 0.5O_2(g) = TiOCl_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	17.197	76.697	76.697	0	-160.000	-157.491	115.442
300	17.219	76.803	76.697	.032	-160.001	-157.474	114.718
400	18.102	81.889	77.384	1.802	-160.031	-156.627	85.576
500	18.630	85.990	78.708	3.641	-160.054	-155.774	68.088
600	18.961	89.418	80.216	5.521	-160.085	-154.916	56.428
700	19.179	92.358	81.745	7.429	-160.132	-154.045	48.094
800	19.329	94.930	83.236	9.355	-160.204	-153.174	41.845
900	19.436	97.213	84.665	11.293	-160.301	-152.288	36.980
1000	19.515	99.265	86.024	13.241	-160.419	-151.391	33.086
1100	19.574	101.128	87.313	15.196	-160.564	-150.487	29.899
1156	19.600	102.100	88.006	16.293	-160.655	-149.969	28.352
1156	19.600	102.100	88.006	16.293	-161.672	-149.969	28.352
1200	19.620	102.833	88.536	17.156	-161.702	-149.522	27.231
1300	19.656	104.405	89.697	19.120	-161.790	-148.504	24.965
1400	19.685	105.863	90.801	21.087	-161.899	-147.479	23.022
1500	19.709	107.222	91.851	23.056	-162.031	-146.444	21.337
1600	19.728	108.494	92.852	25.028	-162.188	-145.400	19.860
1700	19.745	109.691	93.807	27.002	-162.370	-144.343	18.556
1800	19.758	110.820	94.722	28.977	-162.586	-143.279	17.396
1900	19.770	111.888	95.596	30.954	-162.840	-142.196	16.356
1945	19.774	112.351	95.979	31.844	-162.970	-141.706	15.923
1945	19.774	112.351	95.979	31.844	-166.270	-141.706	15.923
2000	19.780	112.903	96.438	32.931	-166.542	-141.010	15.409

*Data estimated.

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.318 + 0.322\times10^{-3}T - 1.970\times10^{5}T^{-2}$
$H°-H°_{298} = 19.318\times10^{-3}T + 0.161\times10^{-6}T^{2} + 1.970\times10^{2}T^{-1} - 6.435$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -160.608 + 1.399\times10^{-3}T - 1.301\times10^{-6}T^{2} + 91.300T^{-1}$
$\Delta Gf° = -160.608 - 1.399\times10^{-3}T\ln T + 1.301\times10^{-6}T^{2} + 45.650T^{-1} + 17.523\times10^{-3}T$
1156-1945 K: $\Delta Hf° = -164.645 + 3.799\times10^{-3}T - 1.624\times10^{-6}T^{2} + 874.200T^{-1}$
$\Delta Gf° = -164.645 - 3.799\times10^{-3}T\ln T + 1.624\times10^{-6}T^{2} + 437.100T^{-1} + 37.275\times10^{-3}T$
1945-2000 K: $\Delta Hf° = -157.513 - 4.174\times10^{-3}T - 0.178\times10^{-6}T^{2} + 106.100T^{-1}$
$\Delta Gf° = -157.513 + 4.174\times10^{-3}T\ln T + 0.178\times10^{-6}T^{2} + 53.050T^{-1} - 23.857\times10^{-3}T$

Sources: Enthalpy of formation at 298 K is that estimated by Monteil (337). Other data are those estimated by JANAF (127).

$TiOF(g)$
Titanium Oxyfluoride (ideal gas)
[Formation: $Ti(c,l) + 0.5F_2(g) + 0.5O_2(g) = TiOF(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.585	59.887	59.887	0	-103.500	-104.646	76.706
300	11.608	59.958	59.888	.021	-103.503	-104.652	76.238
400	12.618	63.447	60.357	1.236	-103.644	-105.013	57.376
500	13.267	66.337	61.271	2.533	-103.757	-105.342	46.045
600	13.690	68.796	62.326	3.882	-103.865	-105.650	38.482
700	13.975	70.929	63.405	5.267	-103.982	-105.931	33.073
800	14.173	72.809	64.466	6.674	-104.118	-106.204	29.013
900	14.315	74.487	65.488	8.099	-104.273	-106.454	25.850
1000	14.420	76.001	66.465	9.536	-104.448	-106.687	23.316
1100	14.500	77.379	67.395	10.982	-104.647	-106.907	21.240
1156	14.535	78.101	67.896	11.796	-104.768	-107.016	20.232
1156	14.535	78.101	67.896	11.796	-105.785	-107.016	20.232
1200	14.562	78.644	68.281	12.436	-105.838	-107.061	19.498
1300	14.611	79.811	69.123	13.894	-105.977	-107.158	18.015
1400	14.650	80.896	69.927	15.357	-106.136	-107.245	16.741
1500	14.682	81.907	70.691	16.824	-106.316	-107.315	15.636
1600	14.708	82.856	71.422	18.294	-106.520	-107.376	14.667
1700	14.730	83.748	72.121	19.766	-106.749	-107.421	13.810
1800	14.749	84.591	72.791	21.240	-107.011	-107.455	13.047
1900	14.764	85.388	73.433	22.715	-107.311	-107.470	12.362
1945	14.770	85.734	73.713	23.380	-107.461	-107.473	12.076
1945	14.770	85.734	73.713	23.380	-110.761	-107.473	12.076
2000	14.778	86.146	74.050	24.192	-111.057	-107.377	11.733

*Data estimated.

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:
$Cp° = 13.942 + 0.592\times10^{-3}T - 2.252\times10^{5}T^{-2}$
$H°-H°_{298} = 13.942\times10^{-3}T + 0.296\times10^{-6}T^{2} + 2.252\times10^{2}T^{-1} - 4.938$

Formation equations (kcal/mol):

298.15-1156 K:
$ΔHf° = -104.035 + 0.596\times10^{-3}T - 1.165\times10^{-6}T^{2} + 137.550T^{-1}$
$ΔGf° = -104.035 - 0.596\times10^{-3}T\ln T + 1.165\times10^{-6}T^{2} + 68.775T^{-1} + 0.227\times10^{-3}T$
1156-1945 K:
$ΔHf° = -108.072 + 2.996\times10^{-3}T - 1.488\times10^{-6}T^{2} + 920.450T^{-1}$
$ΔGf° = -108.072 - 2.996\times10^{-3}T\ln T + 1.488\times10^{-6}T^{2} + 460.225T^{-1} + 19.980\times10^{-3}T$
1945-2000 K:
$ΔHf° = -100.940 - 4.977\times10^{-3}T - 0.042\times10^{-6}T^{2} + 152.350T^{-1}$
$ΔGf° = -100.940 + 4.977\times10^{-3}T\ln T + 0.042\times10^{-6}T^{2} + 76.175T^{-1} - 41.153\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$TiOF_2(g)$
Titanium Oxide Difluoride (ideal gas)
[Formation: $Ti(c,l) + F_2(g) + 0.5O_2(g) = TiOF_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.005	68.016	68.016	0	-221.000	-217.348	159.318
300	15.042	68.109	68.016	.028	-221.003	-217.324	158.318
400	16.625	72.672	68.627	1.618	-221.154	-216.072	118.055
500	17.588	76.494	69.830	3.332	-221.252	-214.792	93.884
600	18.195	79.758	71.218	5.124	-221.332	-213.492	77.763
700	18.597	82.595	72.645	6.965	-221.417	-212.173	66.243
800	18.873	85.097	74.048	8.839	-221.516	-210.848	57.600
900	19.070	87.332	75.402	10.737	-221.635	-209.506	50.874
1000	19.214	89.349	76.698	12.651	-221.772	-208.151	45.491
1100	19.324	91.186	77.933	14.578	-221.934	-206.788	41.084
1156	19.371	92.147	78.598	15.662	-222.033	-206.011	38.947
1156	19.371	92.147	78.598	15.662	-223.050	-206.011	38.947
1200	19.408	92.871	79.109	16.515	-223.087	-205.361	37.401
1300	19.475	94.427	80.228	18.459	-223.187	-203.880	34.275
1400	19.528	95.873	81.294	20.410	-223.309	-202.392	31.594
1500	19.572	97.221	82.311	22.365	-223.451	-200.891	29.269
1600	19.607	98.486	83.284	24.324	-223.619	-199.383	27.234
1700	19.637	99.675	84.213	26.286	-223.812	-197.860	25.436
1800	19.662	100.798	85.103	28.251	-224.039	-196.328	23.837
1900	19.683	101.862	85.958	30.218	-224.304	-194.781	22.405
1945	19.692	102.323	86.331	31.104	-224.439	-194.081	21.808
1945	19.692	102.323	86.331	31.104	-227.739	-194.081	21.808
2000	19.702	102.872	86.779	32.187	-228.017	-193.126	21.104

*Data estimated.

Phase changes: 1156 K, α – β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.709 + 0.716\times10^{-3}T - 3.482\times10^{5}T^{-2}$
$H°-H°_{298} = 18.709\times10^{-3}T + 0.358\times10^{-6}T^{2} + 3.482\times10^{2}T^{-1} - 6.778$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -221.930 + 1.109\times10^{-3}T - 1.191\times10^{-6}T^{2} + 210.300T^{-1}$
$\Delta Gf° = -221.930 - 1.109\times10^{-3}T\ln T + 1.191\times10^{-6}T^{2} + 105.150T^{-1} + 20.150\times10^{-3}T$
1156-1945 K: $\Delta Hf° = -225.967 + 3.509\times10^{-3}T - 1.513\times10^{-6}T^{2} + 993.200T^{-1}$
$\Delta Gf° = -225.967 - 3.509\times10^{-3}T\ln T + 1.513\times10^{-6}T^{2} + 496.600T^{-1} + 39.903\times10^{-3}T$
1945-2000 K: $\Delta Hf° = -218.835 - 4.464\times10^{-3}T - 0.067\times10^{-6}T^{2} + 225.100T^{-1}$
$\Delta Gf° = -218.835 + 4.464\times10^{-3}T\ln T + 0.067\times10^{-6}T^{2} + 112.550T^{-1} - 21.230\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$Tl_2CO_3(c)$
Thallium Carbonate
[Formation: $2Tl(c) + C(c) + 1.5O_2(g) = Tl_2CO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	27.200	37.100	37.100	0	-167.268	-146.857	107.648
300	27.390	37.270	37.103	.050	-167.266	-146.731	106.892
400	35.180	46.280	38.280	3.200	-166.707	-139.955	76.467
473	39.800	52.560	40.002	5.940	-165.966	-135.131	62.437

*Data estimated except enthalpy of formation and entropy at 298 K.

Phase change: 473 K, transition point of Tl_2CO_3; ΔH° unknown.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-473 K: $Cp° = 20.377 + 47.112x10^{-3}T - 6.446x10^{5}T^{-2}$
$H°- H°_{298} = 20.377x10^{-3}T + 23.556x10^{-6}T^{2} + 6.446x10^{2}T^{-1} - 10.331$

Formation equations (kcal/mol):

298.15-473 K: $ΔHf° = -169.859 - 2.038x10^{-3}T + 16.535x10^{-6}T^{2} + 515.300T^{-1}$
$ΔGf° = -169.859 + 2.038x10^{-3}T\ln T - 16.535x10^{-6}T^{2} + 257.650T^{-1} + 67.568x10^{-3}T$

Source: Data from Chang (74) who estimated all except enthalpy of formation and entropy at 298 K.

TlH(g)
Thallium Monohydride (ideal gas)
[Formation: $Tl(c,l,g) + 0.5H_2(g) = TlH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	7.111	51.409	51.409	0	48.906	42.804	-31.376
300	7.115	51.453	51.410	.013	48.900	42.766	-31.155
400	7.376	53.534	51.692	.737	48.636	40.760	-22.270
500	7.672	55.212	52.234	1.489	48.362	38.822	-16.969
507	7.691	55.319	52.276	1.543	48.341	38.690	-16.678
507	7.691	55.319	52.276	1.543	48.251	38.690	-16.678
577	7.880	56.326	52.705	2.089	48.012	37.386	-14.160
577	7.880	56.326	52.705	2.089	47.022	37.386	-14.160
600	7.942	56.635	52.850	2.271	46.960	37.004	-13.478
700	8.168	57.876	53.482	3.076	46.704	35.368	-11.042
800	8.354	58.980	54.101	3.903	46.468	33.759	-9.222
900	8.507	59.973	54.700	4.746	46.245	32.187	-7.816
1000	8.634	60.876	55.273	5.603	46.034	30.638	-6.696
1100	8.742	61.704	55.820	6.472	45.829	29.112	-5.784
1200	8.835	62.469	56.343	7.351	45.631	27.591	-5.025
1300	8.918	63.179	56.841	8.239	45.436	26.099	-4.388
1400	8.993	63.843	57.318	9.135	45.243	24.624	-3.844
1500	9.062	64.466	57.775	10.037	45.052	23.157	-3.374
1600	9.126	65.053	58.211	10.947	44.863	21.707	-2.965
1700	9.188	65.608	58.630	11.863	44.676	20.266	-2.605
1746	9.215	65.854	58.817	12.286	44.590	19.607	-2.454
1746	9.215	65.854	58.817	12.286	5.375	19.607	-2.454
1800	9.246	66.135	59.033	12.784	5.374	20.053	-2.435
1900	9.302	66.636	59.419	13.712	5.368	20.870	-2.401
2000	9.355	67.115	59.792	14.645	5.357	21.686	-2.370

Phase changes: 507 K, α - β transition point of Tl; ΔH° = 0.090 kcal/mol.
577 K, melting point of Tl; ΔH° = 0.990 kcal/mol.
1746 K, boiling point of Tl; ΔH° = 39.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.482 + 1.092\times10^{-3}T - 0.620\times10^{5}T^{-2}$
$H° - H°_{298} = 7.482\times10^{-3}T + 0.546\times10^{-6}T^2 + 0.620\times10^{2}T^{-1} - 2.487$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf° = 48.631 + 0.228\times10^{-3}T - 2.414\times10^{-6}T^2 + 125.650T^{-1}$
$\Delta Gf° = 48.631 - 0.228\times10^{-3}T\ln T + 2.414\times10^{-6}T^2 + 62.825T^{-1} - 19.671\times10^{-3}T$
507-577 K: $\Delta Hf° = 49.487 - 2.237\times10^{-3}T - 0.807\times10^{-6}T^2 + 70.250T^{-1}$
$\Delta Gf° = 49.487 + 2.237\times10^{-3}T\ln T + 0.807\times10^{-6}T^2 + 35.125T^{-1} - 35.790\times10^{-3}T$
577-1746 K: $\Delta Hf° = 48.468 - 2.846\times10^{-3}T + 0.337\times10^{-6}T^2 + 70.250T^{-1}$
$\Delta Gf° = 48.468 + 2.846\times10^{-3}T\ln T - 0.337\times10^{-6}T^2 + 35.125T^{-1} - 37.236\times10^{-3}T$
1746-2000 K: $\Delta Hf° = 5.993 - 0.909\times10^{-3}T + 0.297\times10^{-6}T^2 + 70.250T^{-1}$
$\Delta Gf° = 5.993 + 0.909\times10^{-3}T\ln T - 0.297\times10^{-6}T^2 + 35.125T^{-1} + 1.481\times10^{-3}T$

Source: Data from Gurvich (196).

TlO(g)
Thallium Monoxide (ideal gas)
[Formation: $Tl(c,l,g) + 0.5O_2(g) = TlO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.970	59.136	59.136	0	-46.860	-52.612	38.565
300	7.980	59.185	59.136	.015	-46.864	-52.648	38.353
400	8.465	61.548	59.456	.837	-47.037	-54.551	29.805
500	8.944	63.488	60.072	1.708	-47.209	-56.408	24.655
507	8.976	63.613	60.120	1.771	-47.222	-56.536	24.370
507	8.976	63.613	60.120	1.771	-47.312	-56.536	24.370
577	9.300	64.794	60.618	2.410	-47.478	-57.800	21.893
577	9.300	64.794	60.618	2.410	-48.468	-57.800	21.893
600	9.406	65.160	60.785	2.625	-48.504	-58.170	21.188
700	9.806	66.641	61.517	3.587	-48.641	-59.766	18.659
800	10.113	67.972	62.243	4.583	-48.754	-61.355	16.761
900	10.321	69.176	62.947	5.606	-48.848	-62.920	15.279
1000	10.445	70.271	63.626	6.645	-48.932	-64.478	14.091
1100	10.501	71.269	64.275	7.693	-49.014	-66.024	13.118
1200	10.511	72.184	64.897	8.744	-49.097	-67.576	12.307
1300	10.489	73.024	65.490	9.794	-49.185	-69.110	11.618
1400	10.448	73.800	66.056	10.841	-49.280	-70.634	11.026
1500	10.398	74.519	66.597	11.883	-49.383	-72.156	10.513
1600	10.345	75.189	67.114	12.920	-49.494	-73.669	10.063
1700	10.293	75.814	67.607	13.952	-49.613	-75.176	9.664
1746	10.270	76.089	67.827	14.425	-49.671	-75.866	9.496
1746	10.270	76.089	67.827	14.425	-88.886	-75.866	9.496
1800	10.244	76.401	68.079	14.979	-88.854	-75.457	9.162
1900	10.199	76.954	68.532	16.001	-88.810	-74.715	8.594
2000	10.160	77.476	68.966	17.019	-88.779	-73.972	8.083

*Data except enthalpy of formation at 298 K estimated.

Phase changes:
507 K, α - β transition point of Tl; ΔH° = 0.090 kcal/mol.
577 K, melting point of Tl; ΔH° = 0.990 kcal/mol.
1746 K, boiling point of Tl; ΔH° = 39.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:
$Cp° = 9.571 + 0.668\times10^{-3}T - 1.600\times10^{5}T^{-2}$
$H° - H°_{298} = 9.571\times10^{-3}T + 0.334\times10^{-6}T^{2} + 1.600\times10^{2}T^{-1} - 3.420$

Formation equations (kcal/mol):

298.15-507 K:
$\Delta Hf° = -47.845 + 1.930\times10^{-3}T - 2.668\times10^{-6}T^{2} + 192.800T^{-1}$
$\Delta Gf° = -47.845 - 1.930\times10^{-3}T\ln T + 2.668\times10^{-6}T^{2} + 96.400T^{-1} - 6.873\times10^{-3}T$

507-577 K:
$\Delta Hf° = -46.989 - 0.535\times10^{-3}T - 1.060\times10^{-6}T^{2} + 137.400T^{-1}$
$\Delta Gf° = -46.989 + 0.535\times10^{-3}T\ln T + 1.060\times10^{-6}T^{2} + 68.700T^{-1} - 22.992\times10^{-3}T$

577-1746 K:
$\Delta Hf° = -48.008 - 1.144\times10^{-3}T + 0.083\times10^{-6}T^{2} + 137.400T^{-1}$
$\Delta Gf° = -48.008 + 1.144\times10^{-3}T\ln T - 0.083\times10^{-6}T^{2} + 68.700T^{-1} - 24.438\times10^{-3}T$

1746-2000 K:
$\Delta Hf° = -90.483 + 0.793\times10^{-3}T + 0.043\times10^{-6}T^{2} + 137.400T^{-1}$
$\Delta Gf° = -90.483 - 0.793\times10^{-3}T\ln T - 0.043\times10^{-6}T^{2} + 68.700T^{-1} + 14.279\times10^{-3}T$

Source: Data from Gurvich (196) who estimated all except enthalpy of formation at 298 K.

$TlOH(g)$
Thallium Monohydroxide (ideal gas)
[Formation: $Tl(c,l,g) + 0.5O_2(g) + 0.5H_2(g) = TlOH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	11.641	61.293	61.293	0	-20.000	-21.743	15.938
300	11.655	61.365	61.293	.022	-20.003	-21.754	15.847
400	12.156	64.795	61.757	1.215	-20.153	-22.316	12.193
500	12.419	67.539	62.649	2.445	-20.315	-22.838	9.982
507	12.431	67.712	62.718	2.532	-20.329	-22.872	9.859
507	12.431	67.712	62.718	2.532	-20.419	-22.872	9.859
577	12.548	69.328	63.423	3.407	-20.593	-23.200	8.787
577	12.548	69.328	63.423	3.407	-21.583	-23.200	8.787
600	12.586	69.819	63.659	3.696	-21.626	-23.263	8.474
700	12.718	71.769	64.682	4.961	-21.811	-23.518	7.342
800	12.841	73.475	65.676	6.239	-21.995	-23.756	6.490
900	12.964	74.995	66.629	7.529	-22.177	-23.962	5.819
1000	13.088	76.367	67.535	8.832	-22.357	-24.149	5.278
1100	13.212	77.620	68.395	10.147	-22.534	-24.315	4.831
1200	13.332	78.775	69.213	11.474	-22.709	-24.478	4.458
1300	13.447	79.847	69.991	12.813	-22.881	-24.617	4.138
1400	13.556	80.848	70.732	14.163	-23.051	-24.740	3.862
1500	13.657	81.786	71.437	15.524	-23.219	-24.853	3.621
1600	13.751	82.671	72.112	16.895	-23.385	-24.955	3.409
1700	13.837	83.507	72.758	18.274	-23.550	-25.048	3.220
1746	13.873	83.877	73.046	18.911	-23.626	-25.087	3.140
1746	13.873	83.877	73.046	18.911	-62.841	-25.087	3.140
1800	13.915	84.300	73.377	19.662	-62.829	-23.912	2.903
1900	13.987	85.054	73.971	21.057	-62.815	-21.750	2.502
2000	14.052	85.774	74.545	22.459	-62.807	-19.589	2.141

*Data estimated.

Phase changes: 507 K, α - β transition point of Tl; ΔH° = 0.090 kcal/mol.
577 K, melting point of Tl; ΔH° = 0.990 kcal/mol.
1746 K, boiling point of Tl; ΔH° = 39.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 12.237 + 0.952\times10^{-3}T - 0.782\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 12.237\times10^{-3}T + 0.476\times10^{-6}T^2 + 0.782\times10^{2}T^{-1} - 3.953$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf^\circ = -20.565 + 1.368\times10^{-3}T - 2.735\times10^{-6}T^2 + 119.250T^{-1}$
$\Delta Gf^\circ = -20.565 - 1.368\times10^{-3}T\ln T + 2.735\times10^{-6}T^2 + 59.625T^{-1} + 2.355\times10^{-3}T$
507-577 K: $\Delta Hf^\circ = -19.709 - 1.097\times10^{-3}T - 1.128\times10^{-6}T^2 + 63.850T^{-1}$
$\Delta Gf^\circ = -19.709 + 1.097\times10^{-3}T\ln T + 1.128\times10^{-6}T^2 + 31.925T^{-1} - 13.764\times10^{-3}T$
577-1746 K: $\Delta Hf^\circ = -20.728 - 1.706\times10^{-3}T + 0.015\times10^{-6}T^2 + 63.850T^{-1}$
$\Delta Gf^\circ = -20.728 + 1.706\times10^{-3}T\ln T - 0.015\times10^{-6}T^2 + 31.925T^{-1} - 15.210\times10^{-3}T$
1746-2000 K: $\Delta Hf^\circ = -63.203 + 0.231\times10^{-3}T - 0.025\times10^{-6}T^2 + 63.850T^{-1}$
$\Delta Gf^\circ = -63.203 - 0.231\times10^{-3}T\ln T + 0.025\times10^{-6}T^2 + 31.925T^{-1} + 23.507\times10^{-3}T$

Source: Data are those estimated by Gurvich (196).

$Tl_2SO_4(c,l)$
Thallium Sulfate

[Reaction: $2Tl(c,l) + 0.5S_2(g) + 2O_2(g) = Tl_2SO_4(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	32.045	55.100	55.100	0	-238.155	-208.089	152.531
300	32.151	55.299	55.102	.059	-238.153	-207.902	151.455
400	37.294	65.275	56.428	3.539	-237.774	-197.867	108.108
500	41.852	74.092	59.094	7.499	-237.044	-187.966	82.159
507	42.155	74.676	59.305	7.793	-236.983	-187.277	80.727
507	42.155	74.676	59.305	7.793	-237.163	-187.277	80.727
577	45.185	80.322	61.516	10.851	-236.538	-180.430	68.340
577	45.185	80.322	61.516	10.851	-238.518	-180.430	68.340
600	46.181	82.108	62.271	11.902	-238.243	-178.120	64.879
700	50.400	89.544	65.641	16.732	-236.819	-168.198	52.513
774	53.484	94.762	68.178	20.576	-235.526	-161.022	45.466
774	45.949	94.968	68.178	20.736	-235.366	-161.022	45.466
800	45.238	96.473	69.073	21.920	-235.083	-158.530	43.308
900	48.210	101.894	72.421	26.526	-233.965	-149.018	36.186
916	49.358	102.754	72.944	27.306	-233.746	-147.511	35.194
916	40.000	109.162	72.944	33.176	-227.876	-147.511	35.194
1000	40.000	112.672	76.136	36.536	-227.472	-140.156	30.631

Phase changes:
507 K, α - β transition point of Tl; $\Delta H^\circ = 0.090$ kcal/mol.
577 K, melting point of Tl; $\Delta H^\circ = 0.990$ kcal/mol.
774 K, α - β transition point of Tl_2SO_4; $\Delta H^\circ = 0.160$ kcal/mol.
916 K, melting point of Tl_2SO_4; $\Delta H^\circ = 5.870$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-774 K: $Cp^\circ = 22.442 + 40.594\times10^{-3}T - 2.223\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 22.442\times10^{-3}T + 20.297\times10^{-6}T^{2} + 2.223\times10^{2}T^{-1} - 9.241$
774-916 K: $Cp^\circ = 35.645 + 12.572\times10^{-3}T$
$H^\circ - H^\circ_{298} = 35.645\times10^{-3}T + 6.286\times10^{-6}T^{2} - 10.619$
916-1000 K: $Cp^\circ = 40.000$
$H^\circ - H^\circ_{298} = 40.000\times10^{-3}T - 3.464$

Reaction equations (kcal/mol):

298.15-507 K: $\Delta Hr^\circ = -238.802 - 4.241\times10^{-3}T + 13.631\times10^{-6}T^{2} + 208.550T^{-1}$
$\Delta Gr^\circ = -238.802 + 4.241\times10^{-3}T\ln T - 13.631\times10^{-6}T^{2} + 104.275T^{-1} + 81.736\times10^{-3}T$
507-577 K: $\Delta Hr^\circ = -237.090 - 9.172\times10^{-3}T + 16.845\times10^{-6}T^{2} + 97.750T^{-1}$
$\Delta Gr^\circ = -237.090 + 9.172\times10^{-3}T\ln T - 16.845\times10^{-6}T^{2} + 48.875T^{-1} + 49.498\times10^{-3}T$
577-774 K: $\Delta Hr^\circ = -239.128 - 10.390\times10^{-3}T + 19.131\times10^{-6}T^{2} + 97.750T^{-1}$
$\Delta Gr^\circ = -239.128 + 10.390\times10^{-3}T\ln T - 19.131\times10^{-6}T^{2} + 48.875T^{-1} + 46.606\times10^{-3}T$
774-916 K: $\Delta Hr^\circ = -240.506 + 2.813\times10^{-3}T + 5.120\times10^{-6}T^{2} - 124.550T^{-1}$
$\Delta Gr^\circ = -240.506 - 2.813\times10^{-3}T\ln T - 5.120\times10^{-6}T^{2} - 62.275T^{-1} + 125.548\times10^{-3}T$
916-1000 K: $\Delta Hr^\circ = -233.351 + 7.168\times10^{-3}T - 1.166\times10^{-6}T^{2} - 124.550T^{-1}$
$\Delta Gr^\circ = -233.351 - 7.168\times10^{-3}T\ln T + 1.166\times10^{-6}T^{2} - 62.275T^{-1} + 141.680\times10^{-3}T$

Source: Data from DeKock (113).

TlSe(c,l)
Thallium Selenide
[Reaction: $Tl(c,l) + 0.5Se_2(g) = TlSe(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	11.930	27.560	27.560	0	-31.300	-26.267	19.254
300	11.940	27.634	27.567	.020	-31.301	-26.238	19.114
400	12.150	31.105	28.030	1.230	-31.229	-24.560	13.419
465	12.170	32.937	28.593	2.020	-31.201	-23.478	11.035
465	12.300	33.066	28.593	2.080	-31.141	-23.478	11.035
500	12.300	33.959	28.939	2.510	-31.130	-22.902	10.011
507	12.300	34.130	29.009	2.596	-31.130	-22.787	9.823
507	12.300	34.130	29.009	2.596	-31.220	-22.787	9.823
577	12.300	35.721	29.730	3.457	-31.254	-21.622	8.190
577	12.300	35.721	29.730	3.457	-32.244	-21.622	8.190
600	12.300	36.202	29.969	3.740	-32.240	-21.198	7.721
619	12.300	36.586	30.164	3.975	-32.236	-20.848	7.361
619	18.820	45.100	30.164	9.245	-26.966	-20.848	7.361
700	18.820	47.414	32.028	10.770	-26.425	-20.075	6.268
800	18.820	49.927	34.114	12.650	-25.759	-19.221	5.251

Phase changes: 465 K, α - β transition point of TlSe; ΔH° = 0.060 kcal/mol.
507 K, α - β transition point of Tl; ΔH° = 0.090 kcal/mol.
577 K, melting point of Tl; ΔH° = 0.990 kcal/mol.
619 K, melting point of TlSe; ΔH° = 5.270 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-465 K: $Cp^\circ = 13.782 - 2.562\times10^{-3}T - 0.967\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 13.782\times10^{-3}T - 1.281\times10^{-6}T^2 + 0.967\times10^{2}T^{-1} - 4.320$
465-619 K: $Cp^\circ = 12.305$
$H^\circ - H^\circ_{298} = 12.305\times10^{-3}T - 3.642$
619-800 K: $Cp^\circ = 18.819$
$H^\circ - H^\circ_{298} = 18.819\times10^{-3}T - 2.404$

Reaction equations (kcal/mol):

298.15-465 K: $\Delta Hr^\circ = -32.685 + 4.424\times10^{-3}T - 3.872\times10^{-6}T^2 + 122.150T^{-1}$
$\Delta Gr^\circ = -32.685 - 4.424\times10^{-3}T\ln T + 3.872\times10^{-6}T^2 + 61.075T^{-1} + 44.889\times10^{-3}T$
465-507 K: $\Delta Hr^\circ = -32.007 + 2.947\times10^{-3}T - 2.591\times10^{-6}T^2 + 25.450T^{-1}$
$\Delta Gr^\circ = -32.007 - 2.947\times10^{-3}T\ln T + 2.591\times10^{-6}T^2 + 12.725T^{-1} + 35.179\times10^{-3}T$
507-577 K: $\Delta Hr^\circ = -31.151 + 0.482\times10^{-3}T - 0.983\times10^{-6}T^2 - 29.950T^{-1}$
$\Delta Gr^\circ = -31.151 - 0.482\times10^{-3}T\ln T + 0.983\times10^{-6}T^2 - 14.975T^{-1} + 19.060\times10^{-3}T$
577-619 K: $\Delta Hr^\circ = -32.170 - 0.127\times10^{-3}T + 0.160\times10^{-6}T^2 - 29.950T^{-1}$
$\Delta Gr^\circ = -32.170 + 0.127\times10^{-3}T\ln T - 0.160\times10^{-6}T^2 - 14.975T^{-1} + 17.613\times10^{-3}T$
619-800 K: $\Delta Hr^\circ = -30.932 + 6.387\times10^{-3}T + 0.160\times10^{-6}T^2 - 29.950T^{-1}$
$\Delta Gr^\circ = -30.932 - 6.387\times10^{-3}T\ln T - 0.160\times10^{-6}T^2 - 14.975T^{-1} + 57.486\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (332). Low-temperature heat capacities and entropy at 298 K from Mamedov (323). High-temperature data based on Morgant (339).

$Tl_2Se(c,l)$
Dithallium Selenide
[Reaction: $2Tl(c,l) + 0.5Se_2(g) = Tl_2Se(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	19.650	41.770	41.770	0	-39.150	-33.780	24.761
300	19.670	41.890	41.770	.040	-39.143	-33.743	24.581
400	20.630	47.700	42.550	2.060	-38.903	-31.983	17.474
500	21.350	52.370	44.050	4.160	-38.660	-30.273	13.232
507	21.393	52.667	44.167	4.310	-38.646	-30.154	12.998
507	21.393	52.667	44.167	4.310	-38.826	-30.154	12.998
577	21.827	55.464	45.384	5.816	-38.755	-28.971	10.973
577	21.827	55.464	45.384	5.816	-40.735	-28.971	10.973
600	21.970	56.320	45.787	6.320	-40.674	-28.503	10.382
659	22.310	58.400	46.822	7.630	-40.500	-27.305	9.055
659	27.000	64.470	46.822	11.630	-36.500	-27.305	9.055
700	27.000	66.100	47.900	12.740	-36.179	-26.740	8.348
800	27.000	69.700	50.400	15.440	-35.403	-25.451	6.953
850	27.000	71.340	51.587	16.790	-35.014	-24.838	6.386

Phase changes: 507 K, α - β transition point of Tl; ΔH° = 0.090 kcal/mol.
577 K, melting point of Tl; ΔH° = 0.990 kcal/mol.
659 K, melting point of Tl_2Se; ΔH° = 4.0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-659 K: $Cp° = 19.593 + 4.440x10^{-3}T - 1.126x10^{5}T^{-2}$
$H°- H°_{298} = 19.593x10^{-3}T + 2.220x10^{-6}T^{2} + 1.126x10^{2}T^{-1} - 6.417$
659-850 K: $Cp° = 27.000$
$H°- H°_{298} = 27.000x10^{-3}T - 6.163$

Reaction equations (kcal/mol):

298.15-507 K: $ΔHr° = -41.373 + 6.209x10^{-3}T - 3.121x10^{-6}T^{2} + 193.450T^{-1}$
$ΔGr° = -41.373 - 6.209x10^{-3}TlnT + 3.121x10^{-6}T^{2} + 96.725T^{-1} + 58.823x10^{-3}T$
507-577 K: $ΔHr° = -39.661 + 1.279x10^{-3}T + 0.093x10^{-6}T^{2} + 82.650T^{-1}$
$ΔGr° = -39.661 - 1.279x10^{-3}TlnT - 0.093x10^{-6}T^{2} + 41.325T^{-1} + 26.585x10^{-3}T$
577-659 K: $ΔHr° = -41.699 + 0.061x10^{-3}T + 2.379x10^{-6}T^{2} + 82.650T^{-1}$
$ΔGr° = -41.699 - 0.061x10^{-3}TlnT - 2.379x10^{-6}T^{2} + 41.325T^{-1} + 23.692x10^{-3}T$
659-850 K: $ΔHr° = -41.445 + 7.468x10^{-3}T + 0.160x10^{-6}T^{2} - 29.950T^{-1}$
$ΔGr° = -41.445 - 7.468x10^{-3}TlnT - 0.160x10^{-6}T^{2} - 14.975T^{-1} + 70.051x10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (332). Low-temperature heat capacities and entropy at 298 K from Brekow (56). High-temperature data based on Brekow (56) and Morgant (339).

$Tl_2Te(c,l)$
Dithallium Telluride
[Reaction: $2Tl(c,l) + 0.5Te_2(g) = Tl_2Te(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	18.190	41.600	41.600	0	-38.365	-32.398	23.748
300*	18.200	41.710	41.600	.034	-38.363	-32.360	23.574
400	18.850	47.040	42.325	1.886	-38.233	-30.383	16.600
500	19.500	51.310	43.702	3.804	-38.117	-28.429	12.426
507	19.545	51.581	43.809	3.941	-38.112	-28.292	12.196
507	19.545	51.581	43.809	3.941	-38.292	-28.292	12.196
577	20.000	54.145	44.918	5.324	-38.309	-26.914	10.194
577	20.000	54.145	44.918	5.324	-40.289	-26.914	10.194
600	20.150	54.930	45.287	5.786	-40.259	-26.381	9.609
700	20.800	58.080	46.889	7.834	-40.096	-24.069	7.515
726	20.970	58.850	47.311	8.376	-40.045	-23.480	7.068
726	21.000	66.560	47.311	13.976	-34.445	-23.480	7.068
800	21.000	68.590	49.177	15.530	-34.293	-22.376	6.113

*Data above 298 K estimated except temperature and enthalpy of fusion.

Phase changes: 507 K, α – β transition point of Tl; ΔH° = 0.090 kcal/mol.
577 K, melting point of Tl; ΔH° = 0.990 kcal/mol.
726 K, melting point of Tl_2Te; ΔH° = 5.600 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-726 K: $Cp° = 16.249 + 6.500\times10^{-3}T$
$H°-H°_{298} = 16.249\times10^{-3}T + 3.250\times10^{-6}T^2 - 5.134$
726-800 K: $Cp° = 21.000$
$H°-H°_{298} = 21.000\times10^{-3}T - 1.270$

Reaction equations (kcal/mol):

298.15-507 K: $\Delta Hr° = -39.632 + 3.898\times10^{-3}T - 2.546\times10^{-6}T^2 + 98.700T^{-1}$
$\Delta Gr° = -39.632 - 3.898\times10^{-3}T\ln T + 2.546\times10^{-6}T^2 + 49.350T^{-1} + 45.156\times10^{-3}T$
507-577 K: $\Delta Hr° = -37.920 - 1.032\times10^{-3}T + 0.668\times10^{-6}T^2 - 12.100T^{-1}$
$\Delta Gr° = -37.920 + 1.032\times10^{-3}T\ln T - 0.668\times10^{-6}T^2 - 6.050T^{-1} + 12.918\times10^{-3}T$
577-726 K: $\Delta Hr° = -39.958 - 2.250\times10^{-3}T + 2.954\times10^{-6}T^2 - 12.100T^{-1}$
$\Delta Gr° = -39.958 + 2.250\times10^{-3}T\ln T - 2.954\times10^{-6}T^2 - 6.050T^{-1} + 10.025\times10^{-3}T$
726-800 K: $\Delta Hr° = -36.094 + 2.500\times10^{-3}T - 0.296\times10^{-6}T^2 - 12.100T^{-1}$
$\Delta Gr° = -36.094 - 2.500\times10^{-3}T\ln T + 0.296\times10^{-6}T^2 - 6.050T^{-1} + 33.641\times10^{-3}T$

Source: Data from Mills (332) who estimated all above 298 K except temperature and enthalpy of fusion.

TmO(g)
Thulium Monoxide (ideal gas)
[Formation: Tm(c,l) + 0.5O_2(g) = TmO(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	7.540	60.496	60.496	0	-7.000	-12.457	9.131
300	7.550	60.543	60.496	.014	-7.004	-12.491	9.100
400	7.930	62.770	60.798	.789	-7.233	-14.286	7.806
500	8.200	64.569	61.377	1.596	-7.441	-16.025	7.005
600	8.390	66.082	62.039	2.426	-7.641	-17.724	6.456
700	8.510	67.386	62.712	3.272	-7.851	-19.385	6.052
800	8.600	68.529	63.369	4.128	-8.086	-21.021	5.743
900	8.670	69.547	64.000	4.992	-8.349	-22.620	5.493
1000	8.720	70.462	64.601	5.861	-8.638	-24.185	5.286
1100	8.750	71.295	65.173	6.734	-8.946	-25.732	5.113
1200	8.780	72.058	65.715	7.611	-9.274	-27.242	4.961
1300	8.800	72.761	66.230	8.490	-9.621	-28.723	4.829
1400	8.820	73.415	66.721	9.372	-9.987	-30.172	4.710
1500	8.840	74.024	67.187	10.255	-10.373	-31.609	4.605
1600	8.850	74.595	67.633	11.139	-10.779	-33.012	4.509
1700	8.860	75.132	68.058	12.025	-11.203	-34.383	4.420
1800	8.870	75.639	68.466	12.911	-11.646	-35.744	4.340
1818	8.872	75.727	68.538	13.071	-11.728	-35.978	4.325
1818	8.872	75.727	68.538	13.071	-15.753	-35.978	4.325
1900	8.880	76.118	68.856	13.798	-16.203	-36.885	4.243
2000	8.880	76.573	69.230	14.686	-16.754	-37.953	4.147

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1818 K, melting point of Tm; ΔH° = 4.025 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.485 + 0.264\times10^{-3}T - 0.910\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.485\times10^{-3}T + 0.132\times10^{-6}T^2 + 0.910\times10^{2}T^{-1} - 2.847$

Formation equations (kcal/mol):

298.15-1818 K: $\Delta Hf^\circ = -7.148 - 0.451\times10^{-3}T - 1.153\times10^{-6}T^2 + 114.800T^{-1}$

$\Delta Gf^\circ = -7.148 + 0.451\times10^{-3}T\ln T + 1.153\times10^{-6}T^2 + 57.400T^{-1} - 21.366\times10^{-3}T$

1818-2000 K: $\Delta Hf^\circ = -6.259 - 5.020\times10^{-3}T - 0.119\times10^{-6}T^2 + 68.400T^{-1}$

$\Delta Gf^\circ = -6.259 + 5.020\times10^{-3}T\ln T + 0.119\times10^{-6}T^2 + 34.200T^{-1} - 54.261\times10^{-3}T$

Source: Data from Pedley (396) who estimated all except enthalpy of formation at 298 K.

$UAs_2(c)$
Uranium Diarsenide
[Formation: $U(c) + 2As(\alpha) = UAs_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	19.110	29.410	29.410	0	-60.000	-60.102	44.055
300	19.110	29.530	29.430	.030	-60.004	-60.109	43.789
400	19.470	35.070	30.170	1.960	-59.960	-60.148	32.863
500	19.790	39.440	31.600	3.920	-59.962	-60.193	26.310
600	19.970	43.060	33.210	5.910	-60.023	-60.231	21.939
700	20.240	46.170	34.856	7.920	-60.161	-60.264	18.815

*Enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = 18.375 + 2.744\times10^{-3}T - 0.074\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.375\times10^{-3}T + 1.372\times10^{-6}T^{2} + 0.074\times10^{2}T^{-1} - 5.625$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -61.038 + 3.883\times10^{-3}T - 3.992\times10^{-6}T^{2} + 70.100T^{-1}$

$\Delta Gf^\circ = -61.038 - 3.883\times10^{-3}T\ln T + 3.992\times10^{-6}T^{2} + 35.050T^{-1} + 23.679\times10^{-3}T$

Sources: Data based on Westrum (531) who estimated enthalpy of formation at 298 K.

U_3As_4(c)
Triuranium Tetraarsenide
[Formation: $3U(c) + 4As[\alpha, 1/4As_4(g)] = U_3As_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	44.820	73.870	73.870	0	-172.000	-173.113	126.894
300	44.840	74.150	73.873	.083	-171.997	-173.121	126.117
400	45.630	87.160	75.643	4.607	-171.931	-173.512	94.801
500	46.360	97.420	79.010	9.205	-171.993	-173.900	76.011
600	47.100	105.940	82.815	13.875	-172.222	-174.270	63.477
700	47.810	113.250	86.643	18.625	-172.636	-174.572	54.503
800	48.460	119.700	90.406	23.435	-173.297	-174.831	47.761
876	49.144	124.069	93.084	27.143	-173.972	-174.900	43.635
876	49.144	124.069	93.084	27.143	-207.207	-174.900	43.635
900	49.360	125.400	93.928	28.325	-207.282	-174.014	42.256
942	49.885	127.663	95.382	30.409	-207.445	-172.460	40.011
942	49.885	127.663	95.382	30.409	-209.446	-172.460	40.011
1000	50.610	130.700	97.375	33.325	-209.459	-170.217	37.200

Phase changes: 876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol of $As_4(g)$.
942 K, α − β transition point of U; ΔH° = 0.667 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 42.228 + 7.998\times10^{-3}T + 0.184\times10^{5}T^{-2}$
$H°-H°_{298} = 42.228\times10^{-3}T + 3.999\times10^{-6}T^{2} - 0.184\times10^{2}T^{-1} - 12.884$

Formation equations (kcal/mol):

298.15-876 K: $\Delta Hf° = -174.700 + 10.134\times10^{-3}T - 10.951\times10^{-6}T^{2} + 194.500T^{-1}$
$\Delta Gf° = -174.700 - 10.134\times10^{-3}T\ln T + 10.951\times10^{-6}T^{2} + 97.250T^{-1} + 58.703\times10^{-3}T$
876-942 K: $\Delta Hf° = -212.012 + 12.926\times10^{-3}T - 8.639\times10^{-6}T^{2} + 68.500T^{-1}$
$\Delta Gf° = -212.012 - 12.926\times10^{-3}T\ln T + 8.639\times10^{-6}T^{2} + 34.250T^{-1} + 122.321\times10^{-3}T$
942-1000 K: $\Delta Hf° = -204.782 - 8.509\times10^{-3}T + 4.027\times10^{-6}T^{2} - 194.000T^{-1}$
$\Delta Gf° = -204.782 + 8.509\times10^{-3}T\ln T - 4.027\times10^{-6}T^{2} - 97.000T^{-1} - 20.062\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from Alles (6).

$UB_{1.98}(c)$
Uranium Diboride
[Formation: $U(c,l) + 1.98B(\beta,l) = UB_{1.98}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.230	13.170	13.170	0	-41.600	-41.116	30.139
300	13.290	13.260	13.177	.025	-41.597	-41.113	29.951
400	15.730	17.450	13.733	1.487	-41.449	-40.980	22.390
500	17.260	21.130	14.848	3.141	-41.336	-40.869	17.864
600	18.380	24.380	16.172	4.925	-41.290	-40.787	14.856
700	19.270	27.280	17.553	6.809	-41.300	-40.697	12.706
800	20.010	29.910	18.941	8.775	-41.368	-40.611	11.094
900	20.630	32.300	20.291	10.808	-41.510	-40.504	9.836
942	20.853	33.246	20.848	11.679	-41.596	-40.456	9.386
942	20.853	33.246	20.848	11.679	-42.263	-40.456	9.386
1000	21.160	34.500	21.602	12.898	-42.319	-40.340	8.816
1049	21.381	35.518	22.228	13.940	-42.361	-40.241	8.384
1049	21.381	35.518	22.228	13.940	-43.498	-40.241	8.384
1100	21.610	36.540	22.870	15.037	-43.482	-40.098	7.967
1200	21.980	38.440	24.092	17.217	-43.443	-39.792	7.247
1300	22.290	40.210	25.263	19.431	-43.399	-39.481	6.637
1400	22.530	41.870	26.390	21.672	-43.356	-39.179	6.116
1408	22.545	41.998	26.478	21.852	-43.353	-39.155	6.078
1408	22.545	41.998	26.478	21.852	-45.538	-39.155	6.078
1500	22.720	43.430	27.480	23.935	-45.734	-38.723	5.642
1600	23.320	44.840	28.465	26.200	-45.975	-38.189	5.216
1700	24.090	46.270	29.465	28.568	-46.140	-37.687	4.845
1800	25.130	47.680	30.443	31.027	-46.242	-37.171	4.513
1900	26.480	49.070	31.384	33.604	-46.253	-36.657	4.217
2000	28.200	50.470	32.303	36.335	-46.139	-36.181	3.954
2100	30.340	51.900	33.206	39.258	-45.860	-35.675	3.713
2200	32.950	53.370	34.089	42.418	-45.371	-35.221	3.499
2300	36.080	54.900	34.959	45.865	-44.624	-34.749	3.302
2350	37.940	55.692	35.389	47.710	-44.138	-34.568	3.215
2350	37.940	55.692	35.389	47.710	-67.898	-34.568	3.215
2400	39.800	56.510	35.821	49.654	-67.278	-33.846	3.082
2500	44.140	58.220	36.682	53.845	-65.735	-32.513	2.842

Phase changes:
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.
2350 K, melting point of B; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp^\circ = 15.307 + 6.246\times10^{-3}T - 3.502\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 15.307\times10^{-3}T + 3.123\times10^{-6}T^2 + 3.502\times10^{2}T^{-1} - 6.016$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf^\circ = -42.226 + 2.845\times10^{-3}T - 2.469\times10^{-6}T^2 - 0.870T^{-1}$
$\Delta Gf^\circ = -42.226 - 2.845\times10^{-3}T\ln T + 2.469\times10^{-6}T^2 - 0.435T^{-1} + 19.202\times10^{-3}T$
942-1049 K: $\Delta Hf^\circ = -39.816 - 4.300\times10^{-3}T + 1.753\times10^{-6}T^2 - 88.370T^{-1}$
$\Delta Gf^\circ = -39.816 + 4.300\times10^{-3}T\ln T - 1.753\times10^{-6}T^2 - 44.185T^{-1} - 28.259\times10^{-3}T$
1049-1408 K: $\Delta Hf^\circ = -42.112 - 3.195\times10^{-3}T + 1.753\times10^{-6}T^2 - 88.370T^{-1}$
$\Delta Gf^\circ = -42.112 + 3.195\times10^{-3}T\ln T - 1.753\times10^{-6}T^2 - 44.185T^{-1} - 18.384\times10^{-3}T$
1408-2350 K: $\Delta Hf^\circ = -40.805 - 5.675\times10^{-3}T + 1.753\times10^{-6}T^2 - 88.370T^{-1}$
$\Delta Gf^\circ = -40.805 + 5.675\times10^{-3}T\ln T - 1.753\times10^{-6}T^2 - 44.185T^{-1} - 37.292\times10^{-3}T$
2350-2500 K: $\Delta Hf^\circ = -59.397 - 11.173\times10^{-3}T + 3.123\times10^{-6}T^2 + 350.200T^{-1}$
$\Delta Gf^\circ = -59.397 + 11.173\times10^{-3}T\ln T - 3.123\times10^{-6}T^2 + 175.100T^{-1} - 68.880\times10^{-3}T$

Source: Data from Chiotti (89).

$UB_4(c)$
Uranium Tetraboride
[Formation: $U(c) + 4B(\beta) = UB_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	18.860	17.000	17.000	0	-58.700	-58.509	42.888
300	18.996	17.117	17.000	.035	-58.697	-58.504	42.619
400	24.018	23.359	17.816	2.217	-58.469	-58.481	31.952
500	26.715	29.033	19.503	4.765	-58.285	-58.497	25.568
600	28.498	34.070	21.520	7.530	-58.217	-58.558	21.330
700	29.849	38.568	23.639	10.450	-58.237	-58.607	18.298
800	30.969	42.629	25.763	13.493	-58.331	-58.651	16.023
900	31.956	46.335	27.846	16.640	-58.509	-58.681	14.249
942	32.336	47.801	28.703	17.990	-58.609	-58.687	13.616
942	32.336	47.801	28.703	17.990	-59.276	-58.687	13.616
1000	32.860	49.749	29.868	19.881	-59.355	-58.646	12.817
1049	33.277	51.331	30.834	21.501	-59.413	-58.609	12.210
1049	33.277	51.331	30.834	21.501	-60.550	-58.609	12.210
1100	33.710	52.921	31.821	23.210	-60.548	-58.539	11.631
1200	34.522	55.889	33.704	26.622	-60.527	-58.350	10.627

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 26.800 + 6.950\text{x}10^{-3}T - 8.900\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 26.800\text{x}10^{-3}T + 3.475\text{x}10^{-6}T^{2} + 8.900\text{x}10^{2}T^{-1} - 11.284$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf^\circ = -60.125 + 4.798\text{x}10^{-3}T - 3.515\text{x}10^{-6}T^{2} + 91.500T^{-1}$

$\Delta Gf^\circ = -60.125 - 4.798\text{x}10^{-3}T\ln T + 3.515\text{x}10^{-6}T^{2} + 45.750T^{-1} + 31.194\text{x}10^{-3}T$

942-1049 K: $\Delta Hf^\circ = -57.715 - 2.347\text{x}10^{-3}T + 0.707\text{x}10^{-6}T^{2} + 4.000T^{-1}$

$\Delta Gf^\circ = -57.715 + 2.347\text{x}10^{-3}T\ln T - 0.707\text{x}10^{-6}T^{2} + 2.000T^{-1} - 16.267\text{x}10^{-3}T$

1049-1200 K: $\Delta Hf^\circ = -60.011 - 1.242\text{x}10^{-3}T + 0.707\text{x}10^{-6}T^{2} + 4.000T^{-1}$

$\Delta Gf^\circ = -60.011 + 1.242\text{x}10^{-3}T\ln T - 0.707\text{x}10^{-6}T^{2} + 2.000T^{-1} - 6.392\text{x}10^{-3}T$

Source: Data from Barin (23) who estimated all except enthalpy of formation and entropy at 298 K.

$UB_{12}(c)$
Uranium Dodecaboride
[Formation: $U(c) + 12B(\beta) = UB_{12}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	40.531	33.400	33.400	0	-103.500	-104.836	76.846
300	40.959	33.652	33.402	.075	-103.497	-104.832	76.369
400	56.152	47.821	35.229	5.037	-103.025	-105.366	57.568
500	63.380	61.213	39.109	11.052	-102.630	-105.971	46.320
600	67.474	73.161	43.809	17.611	-102.568	-106.684	38.859
700	70.088	83.772	48.775	24.498	-102.765	-107.338	33.512
800	71.912	93.257	53.753	31.603	-103.165	-107.955	29.492
900	73.279	101.809	58.626	38.865	-103.780	-108.518	26.352
942	73.733	105.162	60.626	41.952	-104.098	-108.733	25.226
942	73.733	105.162	60.626	41.952	-104.765	-108.733	25.226
1000	74.360	109.588	63.339	46.249	-105.187	-108.957	23.812
1049	74.799	113.156	65.583	49.903	-105.562	-109.132	22.736
1049	74.799	113.156	65.583	49.903	-106.699	-109.132	22.736
1100	75.255	116.718	67.872	53.731	-107.059	-109.315	21.719
1200	76.024	123.300	72.220	61.296	-107.837	-109.465	19.936

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 73.750 + 3.700\times10^{-3}T - 30.500\times10^{5}T^{-2}$

$H°-H°_{298} = 73.750\times10^{-3}T + 1.850\times10^{-6}T^{2} + 30.500\times10^{2}T^{-1} - 32.381$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf° = -108.323 + 13.964\times10^{-3}T - 10.676\times10^{-6}T^{2} + 479.500T^{-1}$

$\Delta Gf° = -108.323 - 13.964\times10^{-3}T\ln T + 10.676\times10^{-6}T^{2} + 239.750T^{-1} + 85.376\times10^{-3}T$

942-1049 K: $\Delta Hf° = -105.913 + 6.819\times10^{-3}T - 6.454\times10^{-6}T^{2} + 392.000T^{-1}$

$\Delta Gf° = -105.913 - 6.819\times10^{-3}T\ln T + 6.454\times10^{-6}T^{2} + 196.000T^{-1} + 37.915\times10^{-3}T$

1049-1200 K: $\Delta Hf° = -108.209 + 7.924\times10^{-3}T - 6.454\times10^{-6}T^{2} + 392.000T^{-1}$

$\Delta Gf° = -108.209 - 7.924\times10^{-3}T\ln T + 6.454\times10^{-6}T^{2} + 196.000T^{-1} + 47.790\times10^{-3}T$

Source: Data from Barin (23) who estimated all except enthalpy of formation and entropy at 298 K.

$UBr_5(c)$
Uranium Pentabromide
[Formation: $U(c) + 2.5Br_2(l,g) = UBr_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	38.400	70.000	70.000	0	-193.700	-183.877	134.784
300	38.400	70.238	70.001	.071	-193.723	-183.814	133.907
332.6	38.661	74.213	70.223	1.327	-194.156	-182.716	120.060
332.6	38.661	74.213	70.223	1.327	-211.818	-182.716	120.060
400	39.200	81.394	71.516	3.951	-211.134	-176.891	96.648
500	40.000	90.227	74.405	7.911	-210.116	-168.449	73.628
600	40.800	97.591	77.673	11.951	-209.092	-160.211	58.356
700	41.600	103.940	80.981	16.071	-208.073	-152.144	47.501
800	42.400	109.547	84.208	20.271	-207.064	-144.222	39.399
900	43.200	114.586	87.307	24.551	-206.080	-136.426	33.128
942	43.536	116.564	88.568	26.372	-205.676	-133.186	30.900
942	43.536	116.564	88.568	26.372	-206.343	-133.186	30.900
1000	44.000	119.181	90.270	28.911	-205.705	-128.703	28.128

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 36.000 + 8.000\times10^{-3}T$
$H° - H°_{298} = 36.000\times10^{-3}T + 4.000\times10^{-6}T^2 - 11.089$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -190.318 - 12.338\times10^{-3}T + 0.028\times10^{-6}T^2 + 87.500T^{-1}$
$\Delta Gf° = -190.318 + 12.338\times10^{-3}T\ln T - 0.028\times10^{-6}T^2 + 43.750T^{-1} - 49.175\times10^{-3}T$
332.6-942 K: $\Delta Hf° = -215.319 + 10.565\times10^{-3}T - 0.360\times10^{-6}T^2 + 9.000T^{-1}$
$\Delta Gf° = -215.319 - 10.565\times10^{-3}T\ln T + 0.360\times10^{-6}T^2 + 4.500T^{-1} + 159.212\times10^{-3}T$
942-1000 K: $\Delta Hf° = -212.909 + 3.420\times10^{-3}T + 3.862\times10^{-6}T^2 - 78.500T^{-1}$
$\Delta Gf° = -212.909 - 3.420\times10^{-3}T\ln T - 3.862\times10^{-6}T^2 - 39.250T^{-1} + 111.752\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

UC(c)
Uranium Carbide
[Formation: $U(c,l) + C(c) = UC(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.980	14.150	14.150	0	-23.400	-23.632	17.322
300	12.010	14.220	14.150	.022	-23.394	-23.632	17.216
400	13.190	17.860	14.635	1.290	-23.056	-23.763	12.983
500	13.760	20.870	15.590	2.640	-22.759	-23.976	10.480
600	14.100	23.410	16.687	4.034	-22.539	-24.240	8.829
700	14.360	25.600	17.803	5.458	-22.407	-24.532	7.659
800	14.570	27.540	18.910	6.904	-22.373	-24.847	6.788
900	14.760	29.260	19.959	8.371	-22.442	-25.146	6.106
942	14.840	29.935	20.389	8.993	-22.504	-25.272	5.863
942	14.840	29.935	20.389	8.993	-23.171	-25.272	5.863
1000	14.950	30.830	20.973	9.857	-23.198	-25.405	5.552
1049	15.048	31.548	21.450	10.592	-23.220	-25.512	5.315
1049	15.048	31.548	21.450	10.592	-24.357	-25.512	5.315
1100	15.150	32.260	21.931	11.362	-24.323	-25.554	5.077
1200	15.360	33.590	22.851	12.887	-24.251	-25.684	4.678
1300	15.580	34.830	23.727	14.434	-24.169	-25.810	4.339
1400	15.820	35.990	24.559	16.004	-24.073	-25.934	4.048
1408	15.840	36.080	24.624	16.131	-24.064	-25.944	4.027
1408	15.840	36.080	24.624	16.131	-26.249	-25.944	4.027
1500	16.070	37.090	25.358	17.598	-26.375	-25.920	3.777
1600	16.340	38.140	26.129	19.218	-26.492	-25.894	3.537
1700	16.620	39.130	26.856	20.865	-26.590	-25.840	3.322
1800	16.930	40.090	27.566	22.543	-26.662	-25.794	3.132
1900	17.250	41.020	28.256	24.252	-26.708	-25.756	2.963
2000	17.590	41.910	28.913	25.994	-26.727	-25.699	2.808
2100	17.960	42.780	29.556	27.771	-26.715	-25.654	2.670
2200	18.340	43.620	30.172	29.586	-26.669	-25.595	2.543
2300	18.740	44.450	30.781	31.439	-26.589	-25.561	2.429
2400	19.160	45.250	31.361	33.334	-26.472	-25.505	2.322
2500	19.600	46.040	31.931	35.272	-26.314	-25.464	2.226
2600	20.060	46.820	32.492	37.254	-26.117	-25.441	2.138
2700	20.530	47.590	33.041	39.283	-25.876	-25.431	2.058
2800	21.030	48.340	33.568	41.362	-25.588	-25.403	1.983
2900	21.550	49.090	34.093	43.491	-25.253	-25.410	1.915
3000	22.090	49.830	34.606	45.672	-24.870	-25.425	1.852

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.260 + 1.996\times10^{-3}T - 1.666\times10^{5}T^{-2}$
$H°- H°_{298} = 13.260\times10^{-3}T + 0.998\times10^{-6}T^{2} + 1.666\times10^{2}T^{-1} - 4.601$
2000-3000 K: $Cp° = 4.170 + 5.618\times10^{-3}T + 87.301\times10^{5}T^{-2}$
$H°- H°_{298} = 4.170\times10^{-3}T + 2.809\times10^{-6}T^{2} - 87.301\times10^{2}T^{-1} + 10.783$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf° = -25.297 + 6.632\times10^{-3}T - 3.990\times10^{-6}T^{2} + 81.800T^{-1}$
$\Delta Gf° = -25.297 - 6.632\times10^{-3}T\ln T + 3.990\times10^{-6}T^{2} + 40.900T^{-1} + 41.721\times10^{-3}T$
942-1049 K: $\Delta Hf° = -22.887 - 0.513\times10^{-3}T + 0.232\times10^{-6}T^{2} - 5.700T^{-1}$
$\Delta Gf° = -22.887 + 0.513\times10^{-3}T\ln T - 0.232\times10^{-6}T^{2} - 2.850T^{-1} - 5.740\times10^{-3}T$
1049-1408 K: $\Delta Hf° = -25.183 + 0.592\times10^{-3}T + 0.232\times10^{-6}T^{2} - 5.700T^{-1}$
$\Delta Gf° = -25.183 - 0.592\times10^{-3}T\ln T - 0.232\times10^{-6}T^{2} - 2.850T^{-1} + 4.135\times10^{-3}T$
1408-2000 K: $\Delta Hf° = -23.876 - 1.888\times10^{-3}T + 0.232\times10^{-6}T^{2} - 5.700T^{-1}$
$\Delta Gf° = -23.876 + 1.888\times10^{-3}T\ln T - 0.232\times10^{-6}T^{2} - 2.850T^{-1} - 14.773\times10^{-3}T$
2000-3000 K: $\Delta Hf° = -6.500 - 13.101\times10^{-3}T + 2.675\times10^{-6}T^{2} - 9450.100T^{-1}$
$\Delta Gf° = -6.500 + 13.101\times10^{-3}T\ln T - 2.675\times10^{-6}T^{2} - 4725.050T^{-1} - 102.623\times10^{-3}T$

Source: Data from Tetenbaum (491).

$UC_{1.94}(c)$
Uranium Dicarbide
[Formation: $U(c,l) + 1.94C(c) = UC_{1.94}(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	14.520	16.980	16.980	0	-20.800	-21.491	15.753
300	14.566	17.070	16.980	.027	-20.793	-21.495	15.659
400	16.334	21.540	17.578	1.585	-20.394	-21.790	11.905
500	17.296	25.296	18.756	3.270	-20.060	-22.180	9.695
600	17.963	28.511	20.121	5.034	-19.824	-22.627	8.242
700	18.491	31.321	21.524	6.858	-19.691	-23.105	7.214
800	18.944	33.821	22.908	8.730	-19.663	-23.597	6.446
900	19.353	36.076	24.248	10.645	-19.741	-24.087	5.849
942	19.514	36.962	24.795	11.461	-19.807	-24.289	5.635
942	19.514	36.962	24.795	11.461	-20.474	-24.289	5.635
1000	19.736	38.135	25.535	12.600	-20.505	-24.523	5.359
1049	19.915	39.083	26.146	13.571	-20.530	-24.718	5.150
1049	19.915	39.083	26.146	13.571	-21.667	-24.718	5.150
1100	20.101	40.033	26.768	14.592	-21.635	-24.847	4.936
1200	20.454	41.797	27.947	16.620	-21.566	-25.162	4.583
1300	20.799	43.448	29.077	18.682	-21.486	-25.467	4.281
1400	21.138	45.002	30.160	20.779	-21.389	-25.776	4.024
1408	21.165	45.123	30.245	20.948	-21.380	-25.801	4.005
1408	21.165	45.123	30.245	20.948	-23.565	-25.801	4.005
1500	21.472	46.472	31.199	22.910	-23.688	-25.943	3.780
1600	21.803	47.868	32.197	25.074	-23.800	-26.088	3.563
1700	22.131	49.200	33.159	27.270	-23.896	-26.232	3.372
1800	22.457	50.474	34.085	29.500	-23.968	-26.364	3.201

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1800 K:
$Cp° = 16.932 + 3.110\times10^{-3}T - 2.969\times10^{5}T^{-2}$
$H°- H°_{298} = 16.932\times10^{-3}T + 1.555\times10^{-6}T^{2} + 2.969\times10^{2}T^{-1} - 6.182$

Formation equations (kcal/mol):

298.15-942 K:
$ΔHf° = -22.685 + 6.997\times10^{-3}T - 4.153\times10^{-6}T^{2} + 50.138T^{-1}$
$ΔGf° = -22.685 - 6.997\times10^{-3}T\ln T + 4.153\times10^{-6}T^{2} + 25.069T^{-1} + 42.351\times10^{-3}T$

942-1049 K:
$ΔHf° = -20.275 - 0.148\times10^{-3}T + 0.069\times10^{-6}T^{2} - 37.362T^{-1}$
$ΔGf° = -20.275 + 0.148\times10^{-3}T\ln T - 0.069\times10^{-6}T^{2} - 18.681T^{-1} - 5.110\times10^{-3}T$

1049-1408 K:
$ΔHf° = -22.571 + 0.957\times10^{-3}T + 0.069\times10^{-6}T^{2} - 37.362T^{-1}$
$ΔGf° = -22.571 - 0.957\times10^{-3}T\ln T - 0.069\times10^{-6}T^{2} - 18.681T^{-1} + 4.765\times10^{-3}T$

1408-1800 K:
$ΔHf° = -21.264 - 1.523\times10^{-3}T + 0.069\times10^{-6}T^{2} - 37.362T^{-1}$
$ΔGf° = -21.264 + 1.523\times10^{-3}T\ln T - 0.069\times10^{-6}T^{2} - 18.681T^{-1} - 14.143\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Farr (143). High-temperature data based on Oetting (361) and MacLeod (315).

$U_2C_3(c)$
Diuranium Tricarbide
[Formation: $2U(c,l) + 3C(c) = U_2C_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	25.660	32.930	32.930	0	-43.400	-44.835	32.865
300	25.680	33.100	33.000	.030	-43.406	-44.865	32.684
400	28.670	40.960	33.985	2.790	-42.750	-45.427	24.820
500	29.980	47.510	36.050	5.730	-42.233	-46.158	20.175
600	30.770	53.050	38.433	8.770	-41.918	-46.974	17.110
700	31.420	57.840	40.869	11.880	-41.816	-47.825	14.931
800	32.090	62.080	43.268	15.050	-41.929	-48.685	13.300
900	32.860	65.910	45.577	18.300	-42.238	-49.518	12.024
942	33.234	67.417	46.517	19.688	-42.428	-49.855	11.566
942	33.234	67.417	46.517	19.688	-43.762	-49.855	11.566
1000	33.750	69.410	47.780	21.630	-43.899	-50.218	10.975
1049	34.264	71.037	48.829	23.296	-44.001	-50.523	10.526
1049	34.264	71.037	48.829	23.296	-46.275	-50.523	10.526
1100	34.800	72.680	49.898	25.060	-46.253	-50.701	10.073
1200	36.030	75.760	51.927	28.600	-46.157	-51.143	9.314
1300	37.420	78.690	53.875	32.260	-45.977	-51.568	8.669
1400	39.000	81.530	55.751	36.090	-45.654	-52.011	8.119
1408	39.142	81.753	55.899	36.403	-45.623	-52.048	8.079
1408	39.142	81.753	55.899	36.403	-49.993	-52.048	8.079
1500	40.770	84.280	57.567	40.070	-50.034	-52.187	7.603
1600	42.730	86.970	59.314	44.250	-49.902	-52.321	7.147
1700	44.880	89.620	61.014	48.630	-49.594	-52.477	6.746
1800	47.220	92.250	62.678	53.230	-49.081	-52.659	6.394
1900	49.760	94.870	64.302	58.080	-48.333	-52.874	6.082
2000	52.490	97.490	65.895	63.190	-47.343	-53.137	5.806

Phase changes: 942 K, α − β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β − γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 22.946 + 12.246\times10^{-3}T - 0.833\times10^{5}T^{-2}$
$H°-H°_{298} = 22.946\times10^{-3}T + 6.123\times10^{-6}T^2 + 0.833\times10^{2}T^{-1} - 7.665$

Formation equations (kcal/mol):

298.15-942 K: $ΔHf° = -43.962 + 6.172\times10^{-3}T - 4.619\times10^{-6}T^2 - 258.600T^{-1}$
$ΔGf° = -43.962 - 6.172\times10^{-3}T\ln T + 4.619\times10^{-6}T^2 - 129.300T^{-1} + 32.315\times10^{-3}T$
942-1049 K: $ΔHf° = -39.142 - 8.118\times10^{-3}T + 3.825\times10^{-6}T^2 - 433.600T^{-1}$
$ΔGf° = -39.142 + 8.118\times10^{-3}T\ln T - 3.825\times10^{-6}T^2 - 216.800T^{-1} - 62.607\times10^{-3}T$
1049-1408 K: $ΔHf° = -43.734 - 5.908\times10^{-3}T + 3.825\times10^{-6}T^2 - 433.600T^{-1}$
$ΔGf° = -43.734 + 5.908\times10^{-3}T\ln T - 3.825\times10^{-6}T^2 - 216.800T^{-1} - 42.858\times10^{-3}T$
1408-2000 K: $ΔHf° = -41.121 - 10.868\times10^{-3}T + 3.825\times10^{-6}T^2 - 433.600T^{-1}$
$ΔGf° = -41.121 + 10.868\times10^{-3}T\ln T - 3.825\times10^{-6}T^2 - 216.800T^{-1} - 80.674\times10^{-3}T$

Source: Data from Holley (206).

$UCl_5(c,l)$
Uranium Pentachloride
[Formation: $U(c) + 2.5Cl_2(g) = UCl_5(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	36.000	58.000	58.000	0	-253.000	-226.994	166.389
300	36.020	58.223	58.000	.067	-252.982	-226.832	165.245
400	36.870	68.701	59.423	3.711	-252.100	-218.251	119.245
500	37.720	77.020	62.138	7.441	-251.238	-209.887	91.740
600	38.579	83.973	65.215	11.255	-250.393	-201.697	73.467
600	44.620	98.140	65.215	19.755	-241.893	-201.697	73.467
700	44.620	105.018	70.422	24.217	-240.495	-195.109	60.915
800	44.620	110.976	75.127	28.679	-239.201	-188.718	51.555

*Data except enthalpy of formation at 298 K estimated.

Phase change: 600 K, melting point of UCl_5; ΔH° = 8.500 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 33.500 + 8.432 \times 10^{-3}T$
$H° - H°_{298} = 33.500 \times 10^{-3}T + 4.216 \times 10^{-6}T^2 - 10.363$
600-800 K: $Cp° = 44.620$
$H° - H°_{298} = 44.620 \times 10^{-3}T - 7.017$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = -255.182 + 8.323 \times 10^{-3}T - 0.226 \times 10^{-6}T^2 - 83.250T^{-1}$
$\Delta Gf° = -255.182 - 8.323 \times 10^{-3}T\ln T + 0.226 \times 10^{-6}T^2 - 41.625T^{-1} + 142.363 \times 10^{-3}T$
600-800 K: $\Delta Hf° = -251.836 + 19.443 \times 10^{-3}T - 4.442 \times 10^{-6}T^2 - 83.250T^{-1}$
$\Delta Gf° = -251.836 - 19.443 \times 10^{-3}T\ln T + 4.442 \times 10^{-6}T^2 - 41.625T^{-1} + 205.391 \times 10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

UCl_6(c,l)
Uranium Hexachloride
[Formation: $U(c) + 3Cl_2(g) = UCl_6(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	42.000	68.300	68.300	0	-261.000	-230.121	168.681
300	41.945	68.560	68.300	.078	-260.979	-229.929	167.501
400*	42.020	80.493	69.928	4.226	-260.007	-219.731	120.054
452	44.432	85.757	71.450	6.467	-259.465	-214.525	103.725
452	51.140	96.819	71.450	11.467	-254.465	-214.525	103.725
500	51.140	101.980	74.138	13.921	-253.607	-210.328	91.933
600	51.140	111.304	79.579	19.035	-251.897	-201.835	73.518

*Data above 300 K estimated.

Phase change: 452 K, melting point of UCl_6; ΔH° = 5.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-452 K: $Cp° = 41.866 + 0.448 \times 10^{-3}T$
$H°-H°_{298} = 41.866 \times 10^{-3}T + 0.224 \times 10^{-6}T^2 - 12.502$
452-600 K: $Cp° = 51.140$
$H°-H°_{298} = 51.140 \times 10^{-3}T - 11.648$

Formation equations (kcal/mol):

298.15-452 K: $\Delta Hf° = -263.887 + 12.275 \times 10^{-3}T - 4.262 \times 10^{-6}T^2 - 117.400T^{-1}$
$\Delta Gf° = -263.887 - 12.275 \times 10^{-3}T\ln T + 4.262 \times 10^{-6}T^2 - 58.700T^{-1} + 182.581 \times 10^{-3}T$
452-600 K: $\Delta Hf° = -263.033 + 21.549 \times 10^{-3}T - 4.486 \times 10^{-6}T^2 - 117.400T^{-1}$
$\Delta Gf° = -263.033 - 21.549 \times 10^{-3}T\ln T + 4.486 \times 10^{-6}T^2 - 58.700T^{-1} + 237.289 \times 10^{-3}T$

Source: Data from Fuger (163) who estimated all above 300 K.

UF(g)
Uranium Monofluoride (ideal gas)
[Formation: $U(c,l) + 0.5F_2(g) = UF(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H^\circ_{298})/T$	$H°- H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	9.040	60.340	60.340	0	-10.000	-17.191	12.601
300	9.050	60.396	60.340	.017	-10.002	-17.235	12.556
400	9.580	63.072	60.702	.948	-10.142	-19.627	10.723
500	10.110	65.265	61.401	1.932	-10.295	-21.980	9.607
600	10.740	67.167	62.207	2.976	-10.464	-24.302	8.852
700	10.730	68.822	63.036	4.050	-10.682	-26.590	8.302
800	10.730	70.254	63.851	5.122	-10.993	-28.845	7.880
900	10.740	71.519	64.635	6.196	-11.404	-31.051	7.540
942	10.748	72.009	64.953	6.647	-11.610	-31.964	7.416
942	10.748	72.009	64.953	6.647	-12.277	-31.964	7.416
1000	10.760	72.651	65.380	7.271	-12.504	-33.170	7.249
1049	10.775	73.166	65.732	7.799	-12.695	-34.177	7.120
1049	10.775	73.166	65.732	7.799	-13.832	-34.177	7.120
1100	10.790	73.678	66.089	8.348	-13.976	-35.163	6.986
1200	10.830	74.619	66.762	9.429	-14.256	-37.078	6.753
1300	10.860	75.487	67.399	10.514	-14.533	-38.968	6.551
1400	10.890	76.293	68.007	11.601	-14.811	-40.837	6.375
1408	10.893	76.355	68.054	11.688	-14.833	-40.986	6.362
1408	10.893	76.355	68.054	11.688	-17.018	-40.986	6.362
1500	10.930	77.045	68.584	12.692	-17.500	-42.535	6.197
1600	10.940	77.751	69.135	13.786	-18.021	-44.188	6.036
1700	10.960	78.415	69.661	14.881	-18.544	-45.807	5.889
1800	10.980	79.042	70.165	15.978	-19.066	-47.396	5.755
1900	11.000	79.636	70.648	17.077	-19.586	-48.954	5.631
2000	11.010	80.201	71.112	18.178	-20.107	-50.488	5.517

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.722 + 0.196\times10^{-3}T - 1.547\times10^{5}T^{-2}$
$H°- H^\circ_{298} = 10.722\times10^{-3}T + 0.098\times10^{-6}T^{2} + 1.547\times10^{2}T^{-1} - 3.724$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf° = -11.271 + 3.358\times10^{-3}T - 4.211\times10^{-6}T^{2} + 191.950T^{-1}$
$\Delta Gf° = -11.271 - 3.358\times10^{-3}T\ln T + 4.211\times10^{-6}T^{2} + 95.975T^{-1} - 3.059\times10^{-3}T$
942-1049 K: $\Delta Hf° = -8.861 - 3.787\times10^{-3}T + 0.011\times10^{-6}T^{2} + 104.450T^{-1}$
$\Delta Gf° = -8.861 + 3.787\times10^{-3}T\ln T - 0.011\times10^{-6}T^{2} + 52.225T^{-1} - 50.520\times10^{-3}T$
1049-1408 K: $\Delta Hf° = -11.157 - 2.682\times10^{-3}T + 0.011\times10^{-6}T^{2} + 104.450T^{-1}$
$\Delta Gf° = -11.157 + 2.682\times10^{-3}T\ln T - 0.011\times10^{-6}T^{2} + 52.225T^{-1} - 40.645\times10^{-3}T$
1408-2000 K: $\Delta Hf° = -9.850 - 5.162\times10^{-3}T + 0.011\times10^{-6}T^{2} + 104.450T^{-1}$
$\Delta Gf° = -9.850 + 5.162\times10^{-3}T\ln T - 0.011\times10^{-6}T^{2} + 52.225T^{-1} - 59.553\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

$UF_2(g)$
Uranium Difluoride (ideal gas)
[Formation: $U(c,l) + F_2(g) = UF_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.000	71.180	71.180	0	-127.000	-130.201	95.439
300	16.060	71.279	71.180	.030	-126.996	-130.221	94.865
400	16.190	75.917	71.812	1.642	-126.839	-131.322	71.750
500	16.330	79.545	73.009	3.268	-126.753	-132.454	57.895
600	16.430	82.532	74.355	4.906	-126.742	-133.598	48.662
700	16.530	85.072	75.709	6.554	-126.810	-134.735	42.066
800	16.630	87.286	77.021	8.212	-126.967	-135.859	37.114
900	16.730	89.250	78.272	9.880	-127.219	-136.954	33.257
942	16.772	90.014	78.779	10.584	-127.357	-137.406	31.879
942	16.772	90.014	78.779	10.584	-128.024	-137.406	31.879
1000	16.830	91.018	79.460	11.558	-128.156	-137.981	30.155
1049	16.879	91.824	80.019	12.384	-128.265	-138.459	28.846
1049	16.879	91.824	80.019	12.384	-129.402	-138.459	28.846
1100	16.930	92.627	80.585	13.246	-129.460	-138.898	27.596
1200	17.040	94.104	81.650	14.945	-129.567	-139.750	25.452
1300	17.140	95.472	82.661	16.654	-129.668	-140.594	23.636
1400	17.240	96.746	83.622	18.373	-129.764	-141.432	22.078
1408	17.249	96.844	83.697	18.511	-129.771	-141.498	21.963
1408	17.249	96.844	83.697	18.511	-131.956	-141.498	21.963
1500	17.350	97.939	84.538	20.102	-132.266	-142.112	20.705
1600	17.500	99.064	85.412	21.844	-132.593	-142.759	19.500
1700	17.650	100.129	86.245	23.602	-132.906	-143.383	18.433
1800	17.800	101.142	87.045	25.374	-133.209	-143.991	17.483
1900	17.950	102.109	87.813	27.162	-133.497	-144.582	16.630
2000	18.100	103.033	88.551	28.964	-133.775	-145.159	15.862

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 15.856 + 1.016\times10^{-3}T - 0.141\times10^{5}T^{-2}$
$H°-H°_{298} = 15.856\times10^{-3}T + 0.508\times10^{-6}T^{2} + 0.141\times10^{2}T^{-1} - 4.820$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf° = -127.922 + 4.238\times10^{-3}T - 3.888\times10^{-6}T^{2} + 1.100T^{-1}$
$\Delta Gf° = -127.922 - 4.238\times10^{-3}T\ln T + 3.888\times10^{-6}T^{2} + 0.550T^{-1} + 15.335\times10^{-3}T$
942-1049 K: $\Delta Hf° = -125.512 - 2.907\times10^{-3}T + 0.334\times10^{-6}T^{2} - 86.400T^{-1}$
$\Delta Gf° = -125.512 + 2.907\times10^{-3}T\ln T - 0.334\times10^{-6}T^{2} - 43.200T^{-1} - 32.126\times10^{-3}T$
1049-1408 K: $\Delta Hf° = -127.808 - 1.802\times10^{-3}T + 0.334\times10^{-6}T^{2} - 86.400T^{-1}$
$\Delta Gf° = -127.808 + 1.802\times10^{-3}T\ln T - 0.334\times10^{-6}T^{2} - 43.200T^{-1} - 22.251\times10^{-3}T$
1408-2000 K: $\Delta Hf° = -126.501 - 4.282\times10^{-3}T + 0.334\times10^{-6}T^{2} - 86.400T^{-1}$
$\Delta Gf° = -126.501 + 4.282\times10^{-3}T\ln T - 0.334\times10^{-6}T^{2} - 43.200T^{-1} - 41.159\times10^{-3}T$.

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

$UF_3(g)$
Uranium Trifluoride (ideal gas)
[Formation: $U(c,l) + 1.5F_2(g) = UF_3(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	17.760	79.330	79.330	0	-253.000	-251.410	184.286
300	17.790	79.440	79.330	.033	-253.000	-251.400	183.142
400	20.030	84.912	80.060	1.941	-252.932	-250.873	137.069
500	20.270	89.408	81.496	3.956	-252.859	-250.368	109.434
600	20.510	93.125	83.133	5.995	-252.862	-249.871	91.014
700	20.750	96.304	84.794	8.057	-252.939	-249.367	77.855
800	21.000	99.091	86.410	10.145	-253.098	-248.849	67.981
900	21.240	101.579	87.960	12.257	-253.341	-248.302	60.295
942	21.345	102.550	88.589	13.151	-253.472	-248.065	57.552
942	21.345	102.550	88.589	13.151	-254.139	-248.065	57.552
1000	21.490	103.831	89.436	14.395	-254.258	-247.688	54.132
1049	21.544	104.860	90.133	15.449	-254.356	-247.363	51.535
1049	21.544	104.860	90.133	15.449	-255.493	-247.363	51.535
1100	21.600	105.884	90.839	16.549	-255.539	-246.967	49.067
1200	21.710	107.768	92.172	18.715	-255.625	-246.184	44.836
1300	21.820	109.510	93.440	20.891	-255.706	-245.393	41.254
1400	21.940	111.132	94.647	23.079	-255.783	-244.598	38.183
1408	21.949	111.257	94.741	23.255	-255.789	-244.534	37.956
1408	21.949	111.257	94.741	23.255	-257.974	-244.534	37.956
1500	22.050	112.649	95.796	25.279	-258.266	-243.646	35.499
1600	22.100	114.073	96.894	27.486	-258.581	-242.660	33.145
1700	22.260	115.418	97.945	29.704	-258.888	-241.655	31.067
1800	23.370	116.694	98.952	31.936	-259.186	-240.634	29.217
1900	22.470	117.906	99.919	34.176	-259.479	-239.595	27.559
2000	22.580	119.061	100.846	36.430	-259.764	-238.541	26.066

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.274 + 0.572\times10^{-3}T - 3.276\times10^{5}T^{-2}$
$H°-H°_{298} = 21.274\times10^{-3}T + 0.286\times10^{-6}T^2 + 3.276\times10^{2}T^{-1} - 7.467$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf° = -255.124 + 5.402\times10^{-3}T - 4.197\times10^{-6}T^2 + 264.350T^{-1}$
$\Delta Gf° = -255.124 - 5.402\times10^{-3}T\ln T + 4.197\times10^{-6}T^2 + 132.175T^{-1} + 40.499\times10^{-3}T$
942-1049 K: $\Delta Hf° = -252.714 - 1.743\times10^{-3}T + 0.025\times10^{-6}T^2 + 176.850T^{-1}$
$\Delta Gf° = -252.714 + 1.743\times10^{-3}T\ln T - 0.025\times10^{-6}T^2 + 88.425T^{-1} - 6.962\times10^{-3}T$
1049-1408 K: $\Delta Hf° = -255.010 - 0.638\times10^{-3}T + 0.025\times10^{-6}T^2 + 176.850T^{-1}$
$\Delta Gf° = -255.010 + 0.638\times10^{-3}T\ln T - 0.025\times10^{-6}T^2 + 88.425T^{-1} + 2.913\times10^{-3}T$
1408-2000 K: $\Delta Hf° = -253.703 - 3.118\times10^{-3}T + 0.025\times10^{-6}T^2 + 176.850T^{-1}$
$\Delta Gf° = -253.703 + 3.118\times10^{-3}T\ln T - 0.025\times10^{-6}T^2 + 88.425T^{-1} - 15.995\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

$UF_{4.25}(c)$
Uranium Fluoride
[Formation: $U(c) + 2.125F_2(g) = UF_{4.25}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	29.000	37.700	37.700	0	-469.000	-445.970	326.901
300	29.046	37.880	37.700	.054	-468.988	-445.828	324.781
400	29.832	46.344	38.849	2.998	-468.364	-438.203	239.420
500	30.576	53.081	41.045	6.018	-467.788	-430.730	188.270
600	61.304	58.720	43.532	9.113	-467.254	-423.369	154.210

*Entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 27.100 + 7.080\text{x}10^{-3}T - 0.160\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 27.100\text{x}10^{-3}T + 3.540\text{x}10^{-6}T^{2} + 0.160\text{x}10^{2}T^{-1} - 8.448$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = -470.300 + 5.910\text{x}10^{-3}T - 1.052\text{x}10^{-6}T^{2} - 110.063T^{-1}$

$\Delta Gf° = -470.300 - 5.910\text{x}10^{-3}T\ln T + 1.052\text{x}10^{-6}T^{2} - 55.031T^{-1} + 115.581\text{x}10^{-3}T$

Source: Data from Fuger (163) who estimated entropy at 298 K.

$UF_{4.5}(c)$
Uranium Fluoride
[Formation: $U(c) + 2.25F_2(g) = UF_{4.5}(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	30.000	39.400	39.400	0	-479.900	-455.572	333.939
300	30.059	39.586	39.400	.056	-479.887	-455.421	331.770
400	30.901	48.350	40.590	3.104	-479.256	-447.362	244.424
500	31.676	55.329	42.863	6.233	-478.672	-439.457	192.084
600	32.424	61.171	45.441	9.438	-478.131	-431.666	157.232

*Entropy at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 28.200 + 7.150 \times 10^{-3}T - 0.260 \times 10^{5}T^{-2}$

$H°- H°_{298} = 28.200 \times 10^{-3}T + 3.575 \times 10^{-6}T^{2} + 0.260 \times 10^{2}T^{-1} - 8.813$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = -481.203 + 5.947 \times 10^{-3}T - 1.039 \times 10^{-6}T^{2} - 112.625T^{-1}$

$\Delta Gf° = -481.203 - 5.947 \times 10^{-3}T\ln T + 1.039 \times 10^{-6}T^{2} - 56.313T^{-1} + 120.175 \times 10^{-3}T$

Source:. Data from Fuger (163) who estimated entropy at 298 K.

$UF_5(\alpha,l)$
α-Uranium Pentafluoride
[Formation: $U(c) + 2.5F_2(g) = UF_5(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	31.600	47.700	47.700	0	-496.000	-470.536	344.908
300	31.645	47.896	47.700	.059	-495.988	-470.378	342.666
400	32.590	57.132	48.955	3.271	-495.384	-461.934	252.386
500	33.416	64.493	51.349	6.572	-494.829	-453.635	198.281
600	34.194	70.655	54.068	9.952	-494.322	-445.446	162.252
621	34.358	71.834	54.649	10.672	-494.219	-443.737	156.163
621	39.820	89.869	54.649	21.872	-483.019	-443.737	156.163
700	39.820	94.638	58.898	25.018	-482.243	-438.787	136.994
800	39.820	99.955	63.705	29.000	-481.370	-432.642	118.191
900	39.820	104.645	67.998	32.982	-480.614	-426.595	103.590

Phase change: 621 K, melting point of UF_5; ΔH° = 11.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-621 K: $Cp° = 30.137 + 7.004\times10^{-3}T - 0.556\times10^{5}T^{-2}$

$H°-H°_{298} = 30.137\times10^{-3}T + 3.502\times10^{-6}T^{2} + 0.556\times10^{2}T^{-1} - 9.483$

621-900 K: $Cp° = 39.820$

$H°-H°_{298} = 39.820\times10^{-3}T - 2.856$

Formation equations (kcal/mol):

298.15-621 K: $\Delta Hf° = -497.251 + 5.757\times10^{-3}T - 1.155\times10^{-6}T^{2} - 108.150T^{-1}$

$\Delta Gf° = -497.251 - 5.757\times10^{-3}T\ln T + 1.155\times10^{-6}T^{2} - 54.075T^{-1} + 122.669\times10^{-3}T$

621-900 K: $\Delta Hf° = -490.624 + 15.440\times10^{-3}T - 4.657\times10^{-6}T^{2} - 163.750T^{-1}$

$\Delta Gf° = -490.624 - 15.440\times10^{-3}T\ln T + 4.657\times10^{-6}T^{2} - 81.875T^{-1} + 172.169\times10^{-3}T$

Source: Data from Fuger (163).

$UF_5(\beta,l)$
β-Uranium Pentafluoride
[Formation: $U(c) + 2.5F_2(g) = UF_5(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	31.600	42.900	42.900	0	-497.900	-471.005	345.251
300	31.645	43.096	42.900	.059	-497.888	-470.838	343.001
400	32.590	52.332	44.155	3.271	-497.284	-461.914	252.375
500	33.416	59.693	46.549	6.572	-496.729	-453.135	198.063
600	34.194	65.855	49.268	9.952	-496.221	-444.466	161.895
621	34.358	67.034	49.849	10.672	-496.119	-442.656	155.783
621	39.820	85.069	49.849	21.872	-484.919	-442.656	155.783
700	39.820	89.838	54.098	25.018	-484.143	-437.327	136.538
800	39.820	95.155	58.905	29.000	-483.270	-430.702	117.661
900	39.820	99.845	63.198	32.982	-482.514	-424.175	103.002

Phase change: melting point of UF_5; ΔH° = 11.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-621 K: $Cp° = 30.137 + 7.004x10^{-3}T - 0.556x10^{5}T^{-2}$
$H°- H°_{298} = 30.137x10^{-3}T + 3.502x10^{-6}T^{2} + 0.556x10^{2}T^{-1} - 9.483$
621-900 K: $Cp° = 39.820$
$H°- H°_{298} = 39.820x10^{-3}T - 2.856$

Formation equations (kcal/mol):

298.15-621 K: $\Delta Hf° = -499.151 + 5.757x10^{-3}T - 1.155x10^{-6}T^{2} - 108.150T^{-1}$
$\Delta Gf° = -499.151 - 5.757x10^{-3}TlnT + 1.155x10^{-6}T^{2} - 54.075T^{-1} + 127.469x10^{-3}T$
621-900 K: $\Delta Hf° = -492.524 + 15.440x10^{-3}T - 4.657x10^{-6}T^{2} - 163.750T^{-1}$
$\Delta Gf° = -492.524 - 15.440x10^{-3}TlnT + 4.657x10^{-6}T^{2} - 81.875T^{-1} + 176.969x10^{-3}T$

Source: Data from Fuger (163).

$UF_6(c,l)$
Uranium Hexafluoride
[Formation: $U(c) + 3F_2(g) = UF_6(c,l)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	39.860	54.450	54.450	0	-525.100	-494.427	362.420
300	40.004	54.697	54.450	.074	-525.080	-494.237	360.047
337	43.496	59.573	54.741	1.627	-524.615	-490.457	318.065
337*	45.590	73.091	54.741	6.185	-520.057	-490.457	318.065
400	47.140	81.021	58.266	9.102	-519.045	-485.010	264.994
500	47.400	91.618	63.914	13.852	-517.443	-476.687	208.357

*Heat capacity of liquid estimated.

Phase change: 337 K, melting point of UF_6; $\Delta H^\circ = 4.558$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-337 K: $Cp^\circ = 8.870 + 103.938\times10^{-3}T$

$H^\circ - H^\circ_{298} = 8.870\times10^{-3}T + 51.969\times10^{-6}T^2 - 7.264$

337-500 K: $Cp^\circ = 50.967 - 1.600\times10^{-3}T - 5.494\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 50.967\times10^{-3}T - 0.800\times10^{-6}T^2 + 5.494\times10^{2}T^{-1} - 12.530$

Formation equations (kcal/mol):

298.15-337 K: $\Delta Hf^\circ = -522.688 - 19.764\times10^{-3}T + 47.225\times10^{-6}T^2 - 214.000T^{-1}$

$\Delta Gf^\circ = -522.688 + 19.764\times10^{-3}T\ln T - 47.225\times10^{-6}T^2 - 107.000T^{-1} - 2.536\times10^{-3}T$

337-500 K: $\Delta Hf^\circ = -527.954 + 22.333\times10^{-3}T - 5.544\times10^{-6}T^2 + 335.400T^{-1}$

$\Delta Gf^\circ = -527.954 - 22.333\times10^{-3}T\ln T + 5.544\times10^{-6}T^2 + 167.700T^{-1} + 237.897\times10^{-3}T$

Source: Data from Fuger (163) who estimated heat capacity of liquid.

UN(c)
Uranium Nitride
[Formation: $U(c,l) + 0.5N_2(g) = UN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.370	14.920	14.920	0	-69.500	-63.547	46.581
300	11.390	14.990	14.920	.021	-69.497	-63.510	46.267
400	12.130	18.380	15.380	1.200	-69.353	-61.538	33.622
500	12.620	21.140	16.262	2.439	-69.201	-59.600	26.051
600	13.000	23.480	17.278	3.721	-69.073	-57.695	21.015
700	13.340	25.510	18.313	5.038	-68.987	-55.805	17.423
800	13.660	27.310	19.325	6.388	-68.962	-53.924	14.731
900	13.950	28.930	20.298	7.769	-69.009	-52.035	12.636
942	14.072	29.569	20.697	8.357	-69.056	-51.243	11.889
942	14.072	29.569	20.697	8.357	-69.723	-51.243	11.889
1000	14.240	30.420	21.241	9.179	-69.722	-50.110	10.951
1049	14.377	31.104	21.686	9.880	-69.715	-49.148	10.239
1049	14.377	31.104	21.686	9.880	-70.852	-49.148	10.239
1100	14.520	31.790	22.138	10.617	-70.784	-48.095	9.555
1200	14.800	33.060	22.990	12.084	-70.632	-46.031	8.383
1300	15.080	34.260	23.815	13.578	-70.459	-43.994	7.396
1400	15.350	35.390	24.605	15.099	-70.263	-41.968	6.551
1408	15.372	35.478	24.667	15.222	-70.246	-41.807	6.489
1408	15.372	35.478	24.667	15.222	-72.431	-41.807	6.489
1500	15.630	36.460	25.361	16.648	-72.457	-39.807	5.800
1600	15.900	37.470	26.080	18.224	-72.462	-37.620	5.139
1700	16.170	38.450	26.786	19.828	-72.442	-35.456	4.558
1800*	16.440	39.380	27.459	21.458	-72.399	-33.278	4.040
1900	16.700	40.270	28.104	23.115	-72.332	-31.095	3.577
2000	16.970	41.140	28.740	24.799	-72.240	-28.940	3.162
2100	17.240	41.970	29.346	26.510	-72.123	-26.768	2.786
2200	17.510	42.780	29.940	28.247	-71.981	-24.615	2.445
2300	17.780	43.560	30.511	30.012	-71.813	-22.455	2.134
2400	18.040	44.330	31.079	31.803	-71.621	-20.331	1.851
2500	18.310	45.070	31.622	33.620	-71.404	-18.195	1.591
2600	18.580	45.790	32.151	35.462	-71.163	-16.065	1.350
2700	18.840	46.540	32.713	37.333	-70.894	-14.068	1.139
2800	19.110	47.190	33.179	39.231	-70.600	-11.857	.925
2900	19.380	47.860	33.669	41.155	-70.280	-9.749	.735
3000	19.640	48.520	34.151	43.107	-69.933	-7.665	.558

*Data extrapolated above 1700 K.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $Cp° = 11.681 + 2.658\times10^{-3}T - 0.981\times10^{5}T^{-2}$
$H°-H°_{298} = 11.681\times10^{-3}T + 1.329\times10^{-6}T^{2} + 0.981\times10^{2}T^{-1} - 3.930$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf° = -71.436 + 5.312\times10^{-3}T - 3.187\times10^{-6}T^{2} + 189.550T^{-1}$
$\Delta Gf° = -71.436 - 5.312\times10^{-3}T\ln T + 3.187\times10^{-6}T^{2} + 94.775T^{-1} + 54.711\times10^{-3}T$
942-1049 K: $\Delta Hf° = -69.026 - 1.833\times10^{-3}T + 1.035\times10^{-6}T^{2} + 102.050T^{-1}$
$\Delta Gf° = -69.026 + 1.833\times10^{-3}T\ln T - 1.035\times10^{-6}T^{2} + 51.025T^{-1} + 7.250\times10^{-3}T$
1049-1408 K: $\Delta Hf° = -71.322 - 0.727\times10^{-3}T + 1.035\times10^{-6}T^{2} + 102.050T^{-1}$
$\Delta Gf° = -71.322 + 0.727\times10^{-3}T\ln T - 1.035\times10^{-6}T^{2} + 51.025T^{-1} + 17.125\times10^{-3}T$
1408-2000 K: $\Delta Hf° = -70.016 - 3.208\times10^{-3}T + 1.035\times10^{-6}T^{2} + 102.050T^{-1}$
$\Delta Gf° = -70.016 + 3.208\times10^{-3}T\ln T - 1.035\times10^{-6}T^{2} + 51.025T^{-1} - 1.783\times10^{-3}T$
2000-3000 K: $\Delta Hf° = -68.679 - 4.272\times10^{-3}T + 1.301\times10^{-6}T^{2} - 447.900T^{-1}$
$\Delta Gf° = -68.679 + 4.272\times10^{-3}T\ln T - 1.301\times10^{-6}T^{2} - 223.950T^{-1} - 9.937\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from Oetting (359) who extrapolated data above 1700 K.

UO(g)
Uranium Monoxide (ideal gas)
[Formation: $U(c,l) + 0.5O_2(g) = UO(g)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.570	62.289	62.289	0	6.000	-1.688	1.238
300	7.580	62.336	62.289	.014	5.996	-1.736	1.264
400	7.960	64.571	62.591	.792	5.733	-4.274	2.335
500	8.230	66.380	63.174	1.603	5.442	-6.743	2.947
600	8.410	67.896	63.838	2.435	5.100	-9.148	3.332
700	8.530	69.202	64.513	3.282	4.690	-11.491	3.588
800	8.620	70.348	65.173	4.140	4.196	-13.772	3.762
900	8.680	71.366	65.805	5.005	3.605	-15.982	3.881
942	8.697	71.762	66.062	5.370	3.323	-16.890	3.919
942	8.697	71.762	66.062	5.370	2.656	-16.890	3.919
1000	8.720	72.283	66.408	5.875	2.326	-18.084	3.952
1049	8.740	72.701	66.692	6.303	2.047	-19.076	3.974
1049	8.740	72.701	66.692	6.303	.910	-19.076	3.974
1100	8.760	73.117	66.981	6.750	.675	-20.043	3.982
1200	8.790	73.880	67.524	7.627	.213	-21.906	3.990
1300	8.810	74.585	68.041	8.507	-.250	-23.732	3.990
1400	8.830	75.238	68.532	9.389	-.715	-25.519	3.984
1408	8.831	75.288	68.570	9.460	-.752	-25.661	3.983
1408	8.831	75.288	68.570	9.460	-2.937	-25.661	3.983
1500	8.840	75.848	69.000	10.272	-3.594	-27.126	3.952
1600	8.850	76.419	69.446	11.157	-4.311	-28.672	3.916
1700	8.860	76.956	69.872	12.043	-5.029	-30.172	3.879
1800	8.870	77.463	70.280	12.930	-5.749	-31.629	3.840
1900	8.880	77.943	70.671	13.817	-6.472	-33.048	3.801
2000	8.880	78.399	71.047	14.705	-7.197	-34.430	3.762

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.469 + 0.290\times10^{-3}T - 0.876\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 8.469\times10^{-3}T + 0.145\times10^{-6}T^2 + 0.876\times10^{2}T^{-1} - 2.832$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf^\circ = 5.353 + 1.744\times10^{-3}T - 4.328\times10^{-6}T^2 + 152.500T^{-1}$
$\Delta Gf^\circ = 5.353 - 1.744\times10^{-3}T\ln T + 4.328\times10^{-6}T^2 + 76.250T^{-1} - 15.829\times10^{-3}T$
942-1049 K: $\Delta Hf^\circ = 7.763 - 5.401\times10^{-3}T - 0.106\times10^{-6}T^2 + 65.000T^{-1}$
$\Delta Gf^\circ = 7.763 + 5.401\times10^{-3}T\ln T + 0.106\times10^{-6}T^2 + 32.500T^{-1} - 63.290\times10^{-3}T$
1049-1408 K: $\Delta Hf^\circ = 5.467 - 4.296\times10^{-3}T - 0.106\times10^{-6}T^2 + 65.000T^{-1}$
$\Delta Gf^\circ = 5.467 + 4.296\times10^{-3}T\ln T + 0.106\times10^{-6}T^2 + 32.500T^{-1} - 53.415\times10^{-3}T$
1408-2000 K: $\Delta Hf^\circ = 6.774 - 6.776\times10^{-3}T - 0.106\times10^{-6}T^2 + 65.000T^{-1}$
$\Delta Gf^\circ = 6.774 + 6.776\times10^{-3}T\ln T + 0.106\times10^{-6}T^2 + 32.500T^{-1} - 72.323\times10^{-3}T$

Source: Data from Pedley (396).

$UOBr_2(c)$
Uranium Oxide Bromide
[Formation: $U(c) + 0.5O_2(g) + Br_2(l,g) = UOBr_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	23.420	37.700	37.700	0	-232.700	-222.211	162.883
300	23.480	37.845	37.702	.043	-232.708	-222.145	161.830
332.6*	24.148	40.302	37.838	.819	-232.853	-220.990	145.210
332.6	24.148	40.302	37.838	.819	-239.918	-220.990	145.210
400	25.530	44.903	38.648	2.502	-239.533	-217.193	118.667
500	26.650	50.727	40.499	5.114	-238.904	-211.680	92.524
600	27.410	55.655	42.625	7.818	-238.262	-206.295	75.142
700	28.000	59.926	44.799	10.589	-237.641	-201.017	62.759
800	28.500	63.698	46.929	13.415	-237.063	-195.825	53.496
900	28.930	67.081	48.984	16.287	-236.546	-190.703	46.308

*Data above 300 K estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kca/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp^\circ = 26.318 + 3.406\times10^{-3}T - 3.478\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 26.318\times10^{-3}T + 1.703\times10^{-6}T^2 + 3.478\times10^{2}T^{-1} - 9.165$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -234.295 + 1.502\times10^{-3}T - 2.671\times10^{-6}T^2 + 412.700T^{-1}$

$\Delta Gf^\circ = -234.295 - 1.502\times10^{-3}T\ln T + 2.671\times10^{-6}T^2 + 206.350T^{-1} + 45.970\times10^{-3}T$

332.6-900 K: $\Delta Hf^\circ = -244.295 + 10.663\times10^{-3}T - 2.825\times10^{-6}T^2 + 381.300T^{-1}$

$\Delta Gf^\circ = -244.295 - 10.663\times10^{-3}T\ln T + 2.825\times10^{-6}T^2 + 190.650T^{-1} + 129.325\times10^{-3}T$

Source: Data from Fuger (163) who estimated all above 300 K.

$UOBr_3(c)$
Uranium Oxide Tribromide
[Formation: $U(c) + 0.5O_2(g) + 1.5Br_2(l,g) = UOBr_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	28.900	49.000	49.000	0	-228.000	-215.457	157.932
300	29.010	49.179	49.000	.054	-228.014	-215.377	156.900
332.6	29.691	52.207	49.168	1.011	-228.272	-213.991	140.611
332.6	29.691	52.207	49.168	1.011	-238.870	-213.991	140.611
400	31.100	57.832	50.167	3.066	-238.406	-208.999	114.190
500	32.330	64.910	52.428	6.241	-237.656	-201.732	88.176
600	33.220	70.885	55.020	9.519	-236.884	-194.620	70.889
700	33.960	76.063	57.664	12.879	-236.120	-187.636	58.582
800	34.600	80.640	60.256	16.307	-235.387	-180.761	49.381
900	35.200	84.750	62.753	19.797	-234.702	-173.974	42.246
942	35.452	86.361	63.770	21.281	-234.431	-171.147	39.707
942	35.452	86.361	63.770	21.281	-235.098	-171.147	39.707
1000	35.800	88.490	65.142	23.348	-234.649	-167.223	36.546
1049	36.055	90.209	66.273	25.108	-234.258	-163.927	34.152
1049	36.055	90.209	66.273	25.108	-235.395	-163.927	34.152
1100	36.320	91.927	67.422	26.955	-234.921	-160.464	31.881

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 31.208 + 4.902 \times 10^{-3}T - 3.351 \times 10^{5}T^{-2}$
$H° - H°_{298} = 31.208 \times 10^{-3}T + 2.451 \times 10^{-6}T^{2} + 3.351 \times 10^{2}T^{-1} - 10.646$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -228.384 - 2.653 \times 10^{-3}T - 1.872 \times 10^{-6}T^{2} + 400.000T^{-1}$
$\Delta Gf° = -228.384 + 2.653 \times 10^{-3}T\ln T + 1.872 \times 10^{-6}T^{2} + 200.000T^{-1} + 25.432 \times 10^{-3}T$
332.6-942 K: $\Delta Hf° = -243.385 + 11.088 \times 10^{-3}T - 2.105 \times 10^{-6}T^{2} + 352.900T^{-1}$
$\Delta Gf° = -243.385 - 11.088 \times 10^{-3}T\ln T + 2.105 \times 10^{-6}T^{2} + 176.450T^{-1} + 150.465 \times 10^{-3}T$
942-1049 K: $\Delta Hf° = -240.975 + 3.943 \times 10^{-3}T + 2.117 \times 10^{-6}T^{2} + 265.400T^{-1}$
$\Delta Gf° = -240.975 - 3.943 \times 10^{-3}T\ln T - 2.117 \times 10^{-6}T^{2} + 132.700T^{-1} + 103.004 \times 10^{-3}T$
1049-1100 K: $\Delta Hf° = -243.271 + 5.048 \times 10^{-3}T + 2.117 \times 10^{-6}T^{2} + 265.400T^{-1}$
$\Delta Gf° = -243.271 - 5.048 \times 10^{-3}T\ln T - 2.117 \times 10^{-6}T^{2} + 132.700T^{-1} + 112.879 \times 10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

$UO_2Br_2(c)$
Uranyl Bromide
[Formation: $U(c) + O_2(g) + Br_2(l,g) = UO_2Br_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	27.620	40.500	40.500	0	-271.840	-254.880	186.830
300	27.640	40.671	40.501	.051	-271.847	-254.774	185.600
332.6	27.937	43.538	40.661	.957	-271.977	-252.912	166.185
332.6	27.937	43.538	40.661	.957	-279.042	-252.912	166.185
400	28.550	48.747	41.595	2.861	-278.675	-247.655	135.311
500	29.450	55.215	43.693	5.761	-278.124	-239.964	104.887

*Heat capacity and entropy at 298 K estimated.

Phase change: 332.6 K, boiling point of Br_2 $\Delta H° = 7.065$ kca/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp° = 24.920 + 9.068\times10^{-3}T$

$H°-H°_{298} = 24.920\times10^{-3}T + 4.534\times10^{-6}T^2 - 7.833$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -270.927 - 3.511\times10^{-3}T - 0.091\times10^{-6}T^2 + 42.300T^{-1}$

$\Delta Gf° = -270.927 + 3.511\times10^{-3}T\ln T + 0.091\times10^{-6}T^2 + 21.150T^{-1} + 33.552\times10^{-3}T$

332.6-500 K: $\Delta Hf° = -280.927 + 5.650\times10^{-3}T - 0.246\times10^{-6}T^2 + 10.900T^{-1}$

$\Delta Gf° = -280.927 - 5.650\times10^{-3}T\ln T + 0.246\times10^{-6}T^2 + 5.450T^{-1} + 116.907\times10^{-3}T$

Source: Data from Fuger (163) who estimated heat capacity and entropy at 298 K.

$UOCl_2(c)$
Uranium Oxide Chloride
[Formation: $U(c) + 0.5O_2(g) + Cl_2(g) = UOCl_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	22.720	33.060	33.060	0	-255.000	-238.085	174.519
300	22.780	33.201	33.061	.042	-254.991	-237.980	173.366
400*	24.350	39.982	33.974	2.403	-254.501	-232.383	126.966
500	25.400	45.533	35.747	4.893	-253.966	-226.913	99.182
600	26.190	50.235	37.780	7.473	-253.429	-221.553	80.700
700	26.880	54.323	39.856	10.127	-252.911	-216.280	67.525
800	27.500	57.956	41.899	12.846	-252.430	-211.085	57.665

*Data above 300 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp^\circ = 23.800 + 5.090\times10^{-3}T - 2.380\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 23.800\times10^{-3}T + 2.545\times10^{-6}T^2 + 2.380\times10^{2}T^{-1} - 8.120$

Formation equations (kcal/mol):

298.15-800 K: $\Delta Hf^\circ = -258.067 + 8.248\times10^{-3}T - 2.016\times10^{-6}T^2 + 234.600T^{-1}$

$\Delta Gf^\circ = -258.067 - 8.248\times10^{-3}T\ln T + 2.016\times10^{-6}T^2 + 117.300T^{-1} + 112.091\times10^{-3}T$

Source: Data from Fuger (163) who estimated all above 300 K.

$UOCl_3(c)$
Uranium Oxide Trichloride
[Formation: $U(c) + 0.5O_2(g) + 1.5Cl_2(g) = UOCl_3(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	28.000	41.000	41.000	0	-278.000	-255.508	187.290
300	27.970	41.173	41.000	.052	-277.989	-255.368	186.033
400	28.950	49.354	42.109	2.898	-277.429	-247.914	135.452
500	29.910	55.917	44.235	5.841	-276.867	-240.598	105.164
600	30.870	61.455	46.655	8.880	-276.306	-233.398	85.014
700	31.830	66.286	49.122	12.015	-275.745	-226.290	70.650
800	32.780	70.599	51.543	15.245	-275.196	-219.266	59.900
900	33.740	74.515	53.881	18.571	-274.661	-212.305	51.554

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp^\circ = 25.160 + 9.540\times10^{-3}T - 0.050\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.160\times10^{-3}T + 4.770\times10^{-6}T^{2} + 0.050\times10^{2}T^{-1} - 7.942$

Formation equations (kcal/mol):

298.15-900 K: $\Delta Hf^\circ = -279.454 + 5.194\times10^{-3}T + 0.165\times10^{-6}T^{2} - 32.550T^{-1}$

$\Delta Gf^\circ = -279.454 - 5.194\times10^{-3}T\ln T - 0.165\times10^{-6}T^{2} - 16.275T^{-1} + 110.143\times10^{-3}T$

Source: Data from Fuger (163) who estimated all except enthalpy of formation at 298 K.

UO_2Cl_2(c)
Uranyl Chloride
[Formation: $U(c) + O_2(g) + Cl_2(g) = UO_2Cl_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	25.780	35.980	35.980	0	-297.200	-273.850	200.735
300	25.810	36.140	35.980	.048	-297.192	-273.705	199.391
400	27.170	43.754	37.009	2.698	-296.768	-265.940	145.301
500	28.410	49.951	38.997	5.477	-296.309	-258.285	112.895
600	29.600	55.236	41.273	8.378	-295.829	-250.724	91.325
700	30.760	59.886	43.606	11.396	-295.335	-243.245	75.943
800	31.920	64.069	45.907	14.530	-294.838	-235.840	64.428

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 22.907 + 11.360\times10^{-3}T - 0.457\times10^{5}T^{-2}$

$H°- H°_{298} = 22.907\times10^{-3}T + 5.680\times10^{-6}T^{2} + 0.457\times10^{2}T^{-1} - 7.488$

Formation equations (kcal/mol):

298.15-800 K: $\Delta Hf° = -298.458 + 3.740\times10^{-3}T + 0.867\times10^{-6}T^{2} + 19.700T^{-1}$

$\Delta Gf° = -298.458 - 3.740\times10^{-3}T\ln T - 0.867\times10^{-6}T^{2} + 9.850T^{-1} + 103.992\times10^{-3}T$

Source: Data from Fuger (163).

$UO_2F_2(c)$
Uranyl Fluoride
[Formation: $U(c) + O_2(g) + F_2(g) = UO_2F_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.670	32.400	32.400	0	-395.200	-372.228	272.847
300	24.718	32.553	32.400	.046	-395.193	-372.085	271.060
400	26.787	39.972	33.397	2.630	-394.774	-364.443	199.120

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-400 K: $Cp° = 17.923 + 22.628\times10^{-3}T$

$H°- H°_{298} = 17.923\times10^{-3}T + 11.314\times10^{-6}T^2 - 6.349$

Formation equations (kcal/mol):

298.15-400 K: $\Delta Hf° = -395.299 - 0.925\times10^{-3}T + 6.415\times10^{-6}T^2 - 58.200T^{-1}$

$\Delta Gf° = -395.299 + 0.925\times10^{-3}T\ln T - 6.415\times10^{-6}T^2 - 29.100T^{-1} + 74.351\times10^{-3}T$

Source: Data from Fuger (163).

$UO_2SO_4(\beta)$
β-Uranyl Sulfate
[Reaction: $U(c) + 3O_2(g) + 0.5S_2(g) = UO_2SO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	34.632	39.000	39.000	0	-456.355	-412.447	302.328
300	34.680	39.214	39.001	.064	-456.349	-412.174	300.264
400	37.280	49.547	40.392	3.662	-455.966	-397.504	217.183
500	39.880	58.145	43.105	7.520	-455.451	-382.944	167.382
600	42.480	65.646	46.249	11.638	-454.819	-368.500	134.224
700	45.080	72.390	49.510	16.016	-454.073	-354.170	110.575
800	47.680	78.579	52.762	20.654	-453.217	-339.959	92.871
900	50.280	84.345	55.954	25.552	-452.250	-325.857	79.128
942	51.372	86.663	57.272	27.687	-451.813	-319.970	74.234
942	51.372	86.663	57.272	27.687	-452.480	-319.970	74.234
1000	52.880	89.777	59.067	30.710	-451.752	-311.833	68.150

Phase change: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 26.880 + 26.000 \times 10^{-3}T$

$H° - H°_{298} = 26.880 \times 10^{-3}T + 13.000 \times 10^{-6}T^2 - 9.170$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta Hr° = -456.087 - 2.092 \times 10^{-3}T + 7.109 \times 10^{-6}T^2 - 82.250T^{-1}$

$\Delta Gr° = -456.087 + 2.092 \times 10^{-3}T\ln T - 7.109 \times 10^{-6}T^2 - 41.125T^{-1} + 137.036 \times 10^{-3}T$

942-1000 K: $\Delta Hr° = -453.677 - 9.237 \times 10^{-3}T + 11.331 \times 10^{-6}T^2 - 169.750T^{-1}$

$\Delta Gr° = -453.677 + 9.237 \times 10^{-3}T\ln T - 11.331 \times 10^{-6}T^2 - 84.875T^{-1} + 89.575 \times 10^{-3}T$

Source: Data from Cordfunke (99).

UP(c)
Uranium Phosphide
[Formation: U(c,l) + P(c,l,1/4P_4(g)) = UP(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.860	18.710	18.710	0	-64.000	-63.073	46.233
300	11.880	18.780	18.713	.020	-64.003	-63.068	45.945
317.3	11.980	19.449	18.735	.226	-64.011	-63.013	43.402
317.3	11.980	19.449	18.735	.226	-64.168	-63.013	43.402
400	12.460	22.290	19.190	1.240	-64.245	-62.705	34.260
500	12.870	25.110	20.090	2.510	-64.340	-62.303	27.232
550	13.035	26.349	20.614	3.154	-64.401	-62.117	24.683
550	13.035	26.349	20.614	3.154	-67.309	-62.117	24.683
600	13.200	27.490	21.140	3.810	-67.293	-61.645	22.454
700	13.460	29.540	22.183	5.150	-67.293	-60.692	18.949
800	13.700	31.360	23.235	6.500	-67.374	-59.760	16.325
900	13.910	32.980	24.224	7.880	-67.525	-58.794	14.277
942	13.990	33.616	24.629	8.466	-67.615	-58.385	13.546
942	13.990	33.616	24.629	8.466	-68.282	-58.385	13.546
1000	14.100	34.460	25.170	9.290	-68.335	-57.769	12.625
1049	14.183	35.136	25.620	9.983	-68.382	-57.249	11.927
1049	14.183	35.136	25.620	9.983	-69.519	-57.249	11.927
1100	14.270	35.810	26.083	10.700	-69.518	-56.660	11.257
1200	14.430	37.060	26.943	12.140	-69.482	-55.490	10.106
1300	14.580	38.220	27.766	13.590	-69.437	-54.326	9.133
1400	14.720	39.310	28.560	15.050	-69.383	-53.175	8.301
1408	14.730	39.394	28.621	15.168	-69.378	-53.083	8.239
1408	14.730	39.394	28.621	15.168	-71.563	-53.083	8.239
1500	14.850	40.330	29.310	16.530	-71.723	-51.869	7.557
1600	14.980	41.290	30.021	18.030	-71.878	-50.528	6.902

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to P_4(g); ΔH° = 2.908 kcal/mol of P.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 12.382 + 1.768\times10^{-3}T - 0.932\times10^{5}T^{-2}$
$H° - H°_{298} = 12.382\times10^{-3}T + 0.884\times10^{-6}T^{2} + 0.932\times10^{2}T^{-1} - 4.083$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -65.658 + 5.473\times10^{-3}T - 6.523\times10^{-6}T^{2} + 180.700T^{-1}$
$\Delta Gf° = -65.658 - 5.473\times10^{-3}T\ln T + 6.523\times10^{-6}T^{2} + 90.350T^{-1} + 36.893\times10^{-3}T$
317.3-550 K: $\Delta Hf° = -65.345 + 2.980\times10^{-3}T - 3.338\times10^{-6}T^{2} + 180.700T^{-1}$
$\Delta Gf° = -65.345 - 2.980\times10^{-3}T\ln T + 3.338\times10^{-6}T^{2} + 90.350T^{-1} + 22.556\times10^{-3}T$
550-942 K: $\Delta Hf° = -68.805 + 4.318\times10^{-3}T - 3.342\times10^{-6}T^{2} + 80.400T^{-1}$
$\Delta Gf° = -68.805 - 4.318\times10^{-3}T\ln T + 3.342\times10^{-6}T^{2} + 40.200T^{-1} + 37.454\times10^{-3}T$
942-1049 K: $\Delta Hf° = -66.395 - 2.827\times10^{-3}T + 0.880\times10^{-6}T^{2} - 7.100T^{-1}$
$\Delta Gf° = -66.395 + 2.827\times10^{-3}T\ln T - 0.880\times10^{-6}T^{2} - 3.550T^{-1} - 10.007\times10^{-3}T$
1049-1408 K: $\Delta Hf° = -68.691 - 1.722\times10^{-3}T + 0.880\times10^{-6}T^{2} - 7.100T^{-1}$
$\Delta Gf° = -68.691 + 1.722\times10^{-3}T\ln T - 0.880\times10^{-6}T^{2} - 3.550T^{-1} - 0.132\times10^{-3}T$
1408-1600 K: $\Delta Hf° = -67.384 - 4.202\times10^{-3}T + 0.880\times10^{-6}T^{2} - 7.100T^{-1}$
$\Delta Gf° = -67.384 + 4.202\times10^{-3}T\ln T - 0.880\times10^{-6}T^{2} - 3.550T^{-1} - 19.040\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Low-temperature heat capacities and entropy at 298 K from Counsell (104). High-temperature data based on Chaudhuri (84), Uno (508), and Yokokawa (537).

$USb_2(c)$
Uranium Diantimonide
[Formation: $U(c) + 2Sb(c) = USb_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	19.160	33.810	33.810	0	-42.000	-42.015	30.797
300	19.170	33.930	33.830	.030	-42.004	-42.019	30.610
400	19.840	39.530	34.580	1.980	-41.964	-42.028	22.963
500	20.290	44.010	36.030	3.990	-41.944	-42.044	18.377
600	20.630	47.750	37.683	6.040	-41.971	-42.072	15.325
700	20.800	50.940	39.354	8.110	-42.087	-42.074	13.136

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = 19.153 + 2.756\times10^{-3}T - 0.724\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.153\times10^{-3}T + 1.378\times10^{-6}T^{2} + 0.724\times10^{2}T^{-1} - 6.076$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -43.969 + 5.867\times10^{-3}T - 5.188\times10^{-6}T^{2} + 203.100T^{-1}$

$\Delta Gf^\circ = -43.969 - 5.867\times10^{-3}T\ln T + 5.188\times10^{-6}T^{2} + 101.550T^{-1} + 37.294\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data based on Westrum (531).

U_3Sb_4(c)
Triuranium Tetraantimonide
[Formation: $3U(c) + 4Sb(c) = U_3Sb_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	44.980	83.600	83.600	0	-108.000	-109.216	80.057
300	45.010	83.880	83.603	.083	-107.997	-109.220	79.566
400	46.310	97.010	85.378	4.653	-107.933	-109.638	59.903
500	47.120	107.440	88.786	9.327	-107.975	-110.060	48.107
600	47.860	116.090	92.628	14.077	-108.176	-110.472	40.239
700	48.960	123.600	96.576	18.917	-108.576	-110.846	34.607
800	50.220	130.200	100.354	23.877	-109.219	-111.133	30.360
900	51.460	136.200	104.026	28.957	-110.166	-111.325	27.033

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp° = 42.711 + 9.296\text{x}10^{-3}T - 0.447\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 42.711\text{x}10^{-3}T + 4.648\text{x}10^{-6}T^{2} + 0.447\text{x}10^{2}T^{-1} - 13.297$

Formation equations (kcal/mol):

298.15-900 K: $\Delta Hf° = -112.075 + 13.029\text{x}10^{-3}T - 12.706\text{x}10^{-6}T^{2} + 393.600T^{-1}$

$\Delta Gf° = -112.075 - 13.029\text{x}10^{-3}T\ln T + 12.706\text{x}10^{-6}T^{2} + 196.800T^{-1} + 77.820\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (516). Other data from Alles (6).

USe(c)
Uranium Monoselenide
[Reaction: $U(c,l) + 0.5Se_2(g) = USe(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	13.100	23.070	23.070	0	-82.550	-77.174	56.570
300*	13.110	23.151	23.071	.024	-82.547	-77.141	56.196
400	13.470	26.974	23.589	1.354	-82.401	-75.363	41.176
500	13.750	30.011	24.581	2.715	-82.280	-73.618	32.178
600	13.980	32.538	25.701	4.102	-82.195	-71.894	26.187
700	14.210	34.711	26.837	5.512	-82.158	-70.179	21.911
800	14.400	36.621	27.943	6.942	-82.185	-68.467	18.704
900	14.580	38.327	29.004	8.391	-82.287	-66.747	16.208
942	14.651	38.994	29.434	9.005	-82.356	-66.021	15.317
942	14.651	38.994	29.434	9.005	-83.023	-66.021	15.317
1000	14.750	39.872	30.014	9.858	-83.055	-64.974	14.200
1049	14.823	40.579	30.491	10.583	-83.076	-64.086	13.352
1049	14.823	40.579	30.491	10.583	-84.213	-64.086	13.352
1100	14.900	41.285	30.976	11.340	-84.176	-63.108	12.538
1200	15.060	42.588	31.890	12.838	-84.087	-61.197	11.145
1300	15.210	43.800	32.760	14.352	-83.979	-59.292	9.968
1400	15.360	44.933	33.589	15.881	-83.854	-57.399	8.960
1408	15.371	45.021	33.654	16.004	-83.843	-57.248	8.886
1408	15.371	45.021	33.654	16.004	-86.028	-57.248	8.886
1500	15.500	45.997	34.382	17.423	-86.125	-55.365	8.066
1600	15.650	47.002	35.139	18.981	-86.213	-53.313	7.282
1700	15.800	47.955	35.865	20.553	-86.283	-51.248	6.588
1800	15.950	48.863	36.562	22.141	-86.335	-49.190	5.972
1900	16.100	49.729	37.233	23.743	-86.369	-47.126	5.421
2000	16.250	50.559	37.878	25.361	-86.384	-45.064	4.924

*Data above 298 K estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.208 + 1.552\times10^{-3}T - 0.508\times10^{5}T^{-2}$
$H°-H°_{298} = 13.208\times10^{-3}T + 0.776\times10^{-6}T^{2} + 0.508\times10^{2}T^{-1} - 4.177$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta Hr° = -84.042 + 4.766\times10^{-3}T - 3.286\times10^{-6}T^{2} + 108.350T^{-1}$
$\Delta Gr° = -84.042 - 4.766\times10^{-3}T\ln T + 3.286\times10^{-6}T^{2} + 54.175T^{-1} + 48.600\times10^{-3}T$
942-1049 K: $\Delta Hr° = -81.632 - 2.379\times10^{-3}T + 0.936\times10^{-6}T^{2} + 20.850T^{-1}$
$\Delta Gr° = -81.632 + 2.379\times10^{-3}T\ln T - 0.936\times10^{-6}T^{2} + 10.425T^{-1} + 1.139\times10^{-3}T$
1049-1408 K: $\Delta Hr° = -83.928 - 1.274\times10^{-3}T + 0.936\times10^{-6}T^{2} + 20.850T^{-1}$
$\Delta Gr° = -83.928 + 1.274\times10^{-3}T\ln T - 0.936\times10^{-6}T^{2} + 10.425T^{-1} + 11.014\times10^{-3}T$
1408-2000 K: $\Delta Hr° = -82.622 - 3.754\times10^{-3}T + 0.936\times10^{-6}T^{2} + 20.850T^{-1}$
$\Delta Gr° = -82.622 + 3.754\times10^{-3}T\ln T - 0.936\times10^{-6}T^{2} + 10.425T^{-1} - 7.894\times10^{-3}T$

Source: Data from Gronvold (187) who estimated all above 298 K.

USe(g)
Uranium Monoselenide (ideal gas)
[Reaction: U(c,l) + 0.5Se_2(g) = USe(g)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	8.751	65.640	65.640	0	68.350	61.033	-44.738
300	8.755	65.694	65.641	.016	68.345	60.988	-44.429
400	8.981	68.244	65.987	.903	68.049	58.578	-32.005
500	9.194	70.271	66.647	1.812	67.717	56.249	-24.586
600	9.385	71.965	67.397	2.741	67.344	53.989	-19.665
700	9.548	73.424	68.155	3.688	66.918	51.798	-16.172
800	9.683	74.708	68.896	4.650	66.423	49.672	-13.570
900	9.794	75.855	69.606	5.624	65.846	47.611	-11.561
942	9.831	76.303	69.895	6.036	65.575	46.766	-10.850
942	9.831	76.303	69.895	6.036	64.908	46.766	-10.850
1000	9.882	76.892	70.284	6.608	64.596	45.657	-9.978
1049	9.915	77.366	70.604	7.093	64.335	44.736	-9.320
1049	9.915	77.366	70.604	7.093	63.198	44.736	-9.320
1100	9.950	77.837	70.928	7.600	62.984	43.845	-8.711
1200	10.001	78.705	71.541	8.597	62.573	42.122	-7.671
1300	10.036	79.507	72.123	9.599	62.168	40.436	-6.798
1400	10.057	80.252	72.678	10.604	61.770	38.777	-6.053
1408	10.058	80.309	72.721	10.684	61.738	38.646	-5.999
1408	10.058	80.309	72.721	10.684	59.553	38.646	-5.999
1500	10.067	80.946	73.206	11.610	58.962	37.299	-5.434
1600	10.067	81.596	73.710	12.617	58.323	35.872	-4.900
1700	10.059	82.206	74.192	13.623	57.687	34.496	-4.435
1800	10.044	82.781	74.654	14.629	57.053	33.146	-4.024
1900	10.025	83.323	75.096	15.632	56.420	31.834	-3.662
2000	10.001	83.837	75.521	16.633	55.788	30.552	-3.339

*Data estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.219 + 0.600 \times 10^{-3}T - 0.575 \times 10^{5}T^{-2}$
$H°- H°_{298} = 9.219 \times 10^{-3}T + 0.300 \times 10^{-6}T^{2} + 0.575 \times 10^{2}T^{-1} - 2.968$

Reaction equations (kcal/mol):

298.15-942 K: $ΔHr° = 68.067 + 0.777 \times 10^{-3}T - 3.763 \times 10^{-6}T^{2} + 115.050T^{-1}$
$ΔGr° = 68.067 - 0.777 \times 10^{-3}T\ln T + 3.763 \times 10^{-6}T^{2} + 57.525T^{-1} - 20.932 \times 10^{-3}T$
942-1049 K: $ΔHr° = 70.477 - 6.368 \times 10^{-3}T + 0.460 \times 10^{-6}T^{2} + 27.550T^{-1}$
$ΔGr° = 70.477 + 6.368 \times 10^{-3}T\ln T - 0.460 \times 10^{-6}T^{2} + 13.775T^{-1} - 68.393 \times 10^{-3}T$
1049-1408 K: $ΔHr° = 68.181 - 5.263 \times 10^{-3}T + 0.460 \times 10^{-6}T^{2} + 27.550T^{-1}$
$ΔGr° = 68.181 + 5.263 \times 10^{-3}T\ln T - 0.460 \times 10^{-6}T^{2} + 13.775T^{-1} - 58.519 \times 10^{-3}T$
1408-2000 K: $ΔHr° = 69.488 - 7.743 \times 10^{-3}T + 0.460 \times 10^{-6}T^{2} + 27.550T^{-1}$
$ΔGr° = 69.488 + 7.743 \times 10^{-3}T\ln T - 0.460 \times 10^{-6}T^{2} + 13.775T^{-1} - 77.427 \times 10^{-3}T$

Source: Data are those estimated by Gronvold (187).

$USe_{1.5}(c)$
Uranium Sesquiselenide
[Reaction: $U(c,l) + 0.75Se_2(g) = USe_{1.5}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	16.030	32.200	32.200	0	-109.975	-102.983	75.488
300	16.050	32.299	32.200	.030	-109.971	-102.939	74.990
400	16.470	36.977	32.835	1.657	-109.776	-100.627	54.979
500	16.780	40.686	34.048	3.319	-109.606	-98.360	42.993
600	17.060	43.771	35.418	5.012	-109.468	-96.126	35.013
700	17.280	46.417	36.804	6.729	-109.377	-93.907	29.319
800	17.500	48.739	38.154	8.468	-109.346	-91.698	25.051
900	17.690	50.811	39.447	10.228	-109.389	-89.491	21.731
942	17.770	51.620	39.971	10.973	-109.432	-88.562	20.547
942	17.770	51.620	39.971	10.973	-110.099	-88.562	20.547
1000	17.880	52.685	40.679	12.006	-110.095	-87.239	19.066
1049	17.958	53.542	41.260	12.884	-110.085	-86.119	17.942
1049	17.958	53.542	41.260	12.884	-111.222	-86.119	17.942
1100	18.040	54.397	41.850	13.802	-111.150	-84.899	16.868
1200	18.200	55.973	42.961	15.614	-110.994	-82.518	15.028
1300	18.360	57.436	44.019	17.442	-110.819	-80.150	13.474
1400	18.530	58.803	45.027	19.287	-110.621	-77.800	12.145
1408	18.542	58.909	45.105	19.435	-110.604	-77.613	12.047
1408	18.542	58.909	45.105	19.435	-112.789	-77.613	12.047
1500	18.680	60.087	45.989	21.147	-112.818	-75.315	10.973
1600	18.840	61.298	46.909	23.023	-112.828	-72.819	9.946
1700	19.010	62.445	47.789	24.916	-112.817	-70.306	9.038
1800	19.170	63.536	48.633	26.825	-112.786	-67.812	8.233
1900	19.340	64.577	49.445	28.750	-112.735	-65.318	7.513
2000	19.500	65.573	50.227	30.692	-112.661	-62.828	6.865

*Enthalpy of formation at 298 K and all data above 298 K estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.248 + 1.648\times10^{-3}T - 0.631\times10^{5}T^{-2}$
$H°-H°_{298} = 16.248\times10^{-3}T + 0.824\times10^{-6}T^2 + 0.631\times10^{2}T^{-1} - 5.129$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta Hr° = -111.581 + 5.140\times10^{-3}T - 3.159\times10^{-6}T^2 + 105.675T^{-1}$
$\Delta Gr° = -111.581 - 5.140\times10^{-3}T\ln T + 3.159\times10^{-6}T^2 + 52.838T^{-1} + 56.586\times10^{-3}T$
942-1049 K: $\Delta Hr° = -109.171 - 2.005\times10^{-3}T + 1.063\times10^{-6}T^2 + 18.175T^{-1}$
$\Delta Gr° = -109.171 + 2.005\times10^{-3}T\ln T - 1.063\times10^{-6}T^2 + 9.087T^{-1} + 9.125\times10^{-3}T$
1049-1408 K: $\Delta Hr° = -111.467 - 0.900\times10^{-3}T + 1.063\times10^{-6}T^2 + 18.175T^{-1}$
$\Delta Gr° = -111.467 + 0.900\times10^{-3}T\ln T - 1.063\times10^{-6}T^2 + 9.087T^{-1} + 19.000\times10^{-3}T$
1408-2000 K: $\Delta Hr° = -110.160 - 3.380\times10^{-3}T + 1.063\times10^{-6}T^2 + 18.175T^{-1}$
$\Delta Gr° = -110.160 + 3.380\times10^{-3}T\ln T - 1.063\times10^{-6}T^2 + 9.087T^{-1} + 0.092\times10^{-3}T$

Source: Data from Gronvold (187) who estimated enthalpy of formation at 298 K and all data above 298 K.

$USe_2(c)$
Uranium Diselenide
[Reaction: $U(c,l) + Se_2(g) = USe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	18.920	32.260	32.260	0	-135.300	-123.988	90.885
300	19.000	32.377	32.260	.035	-135.295	-123.918	90.273
400	19.470	37.910	33.010	1.960	-135.051	-120.163	65.653
500	19.820	42.293	34.445	3.924	-134.831	-116.467	50.907
600	20.130	45.936	36.064	5.923	-134.640	-112.815	41.092
700	20.360	49.056	37.703	7.947	-134.494	-109.187	34.089
800	20.600	51.791	39.297	9.995	-134.407	-105.577	28.842
900	20.800	54.229	40.823	12.065	-134.390	-101.976	24.763
942	20.884	55.180	41.442	12.940	-134.408	-100.464	23.308
942	20.884	55.180	41.442	12.940	-135.075	-100.464	23.308
1000	21.000	56.431	42.276	14.155	-135.034	-98.337	21.491
1049	21.088	57.438	42.961	15.186	-134.993	-96.539	20.113
1049	21.088	57.438	42.961	15.186	-136.130	-96.539	20.113
1100	21.180	58.441	43.655	16.265	-136.024	-94.613	18.798
1200	21.350	60.291	44.965	18.391	-135.801	-90.859	16.547
1300	21.520	62.006	46.210	20.535	-135.555	-87.118	14.646
1400	21.690	63.608	47.397	22.695	-135.287	-83.409	13.021
1408	21.703	63.732	47.490	22.869	-135.264	-83.112	12.900
1408	21.703	63.732	47.490	22.869	-137.449	-83.112	12.900
1500	21.850	65.109	48.528	24.872	-137.409	-79.562	11.592
1600	22.030	66.525	49.609	27.066	-137.343	-75.713	10.342
1700	22.210	67.866	50.644	29.278	-137.253	-71.849	9.237
1800	22.390	69.141	51.637	31.508	-137.139	-68.014	8.258
1900	22.570	70.356	52.590	33.756	-137.001	-64.180	7.382
2000	22.750	71.518	53.507	36.022	-136.838	-60.356	6.595

*Enthalpy of formation at 298 K and all data above 298 K estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.323 + 1.724\times10^{-3}T - 0.815\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 19.323\times10^{-3}T + 0.862\times10^{-6}T^2 + 0.815\times10^{2}T^{-1} - 6.111$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta Hr^\circ = -137.050 + 5.549\times10^{-3}T - 3.041\times10^{-6}T^2 + 109.100T^{-1}$
$\Delta Gr^\circ = -137.050 - 5.549\times10^{-3}T\ln T + 3.041\times10^{-6}T^2 + 54.550T^{-1} + 73.905\times10^{-3}T$
942-1049 K: $\Delta Hr^\circ = -134.640 - 1.596\times10^{-3}T + 1.181\times10^{-6}T^2 + 21.600T^{-1}$
$\Delta Gr^\circ = -134.640 + 1.596\times10^{-3}T\ln T - 1.181\times10^{-6}T^2 + 10.800T^{-1} + 26.444\times10^{-3}T$
1049-1408 K: $\Delta Hr^\circ = -136.936 - 0.491\times10^{-3}T + 1.181\times10^{-6}T^2 + 21.600T^{-1}$
$\Delta Gr^\circ = -136.936 + 0.491\times10^{-3}T\ln T - 1.181\times10^{-6}T^2 + 10.800T^{-1} + 36.319\times10^{-3}T$
1408-2000 K: $\Delta Hr^\circ = -135.629 - 2.971\times10^{-3}T + 1.181\times10^{-6}T^2 + 21.600T^{-1}$
$\Delta Gr^\circ = -135.629 + 2.971\times10^{-3}T\ln T - 1.181\times10^{-6}T^2 + 10.800T^{-1} + 17.411\times10^{-3}T$

Source: Data from Gronvold (187) who estimated enthalpy of formation at 298 K and all data above 298 K.

$USe_2(g)$
Uranium Diselenide (ideal gas)
[Reaction: $U(c,l) + Se_2(g) = USe_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	14.401	74.720	74.720	0	17.700	16.352	-11.986
300	14.406	74.809	74.720	.027	17.697	16.345	-11.907
400	14.616	78.985	75.287	1.479	17.468	15.926	-8.701
500	14.717	82.258	76.366	2.946	17.191	15.572	-6.806
600	14.773	84.946	77.579	4.420	16.857	15.276	-5.564
700	14.807	87.226	78.799	5.899	16.458	15.046	-4.698
800	14.830	89.205	79.979	7.381	15.979	14.878	-4.064
900	14.845	90.953	81.103	8.865	15.410	14.772	-3.587
942	14.850	91.630	81.557	9.489	15.141	14.748	-3.422
942	14.850	91.630	81.557	9.489	14.474	14.748	-3.422
1000	14.856	92.518	82.168	10.350	14.161	14.771	-3.228
1049	14.860	93.229	82.668	11.078	13.899	14.808	-3.085
1049	14.860	93.229	82.668	11.078	12.762	14.808	-3.085
1100	14.864	93.934	83.174	11.836	12.547	14.915	-2.963
1200	14.871	95.227	84.124	13.323	12.131	15.150	-2.759
1300	14.876	96.418	85.026	14.810	11.720	15.421	-2.592
1400	14.880	97.521	85.880	16.298	11.316	15.716	-2.453
1408	14.880	97.606	85.946	16.417	11.284	15.741	-2.443
1408	14.880	97.606	85.946	16.417	9.099	15.741	-2.443
1500	14.883	98.547	86.690	17.786	8.505	16.196	-2.360
1600	14.885	99.508	87.461	19.275	7.866	16.724	-2.284
1700	14.887	100.410	88.196	20.763	7.232	17.311	-2.225
1800	14.889	101.261	88.899	22.252	6.605	17.914	-2.175
1900	14.891	102.066	89.571	23.741	5.984	18.556	-2.134
2000	14.892	102.830	90.215	25.230	5.370	19.228	-2.101

*Data estimated.

Phase changes:
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:
$Cp° = 14.882 + 0.014 \times 10^{-3}T - 0.431 \times 10^{5}T^{-2}$
$H°- H°_{298} = 14.882 \times 10^{-3}T + 0.007 \times 10^{-6}T^{2} + 0.431 \times 10^{2}T^{-1} - 4.582$

Reaction equations (kcal/mol):

298.15-942 K:
$\Delta Hr° = 17.479 + 1.108 \times 10^{-3}T - 3.896 \times 10^{-6}T^{2} + 70.700T^{-1}$
$\Delta Gr° = 17.479 - 1.108 \times 10^{-3}T\ln T + 3.896 \times 10^{-6}T^{2} + 35.350T^{-1} + 0.975 \times 10^{-3}T$

942-1049 K:
$\Delta Hr° = 19.889 - 6.037 \times 10^{-3}T + 0.326 \times 10^{-6}T^{2} - 16.800T^{-1}$
$\Delta Gr° = 19.889 + 6.037 \times 10^{-3}T\ln T - 0.326 \times 10^{-6}T^{2} - 8.400T^{-1} - 46.486 \times 10^{-3}T$

1049-1408 K:
$\Delta Hr° = 17.593 - 4.932 \times 10^{-3}T + 0.326 \times 10^{-6}T^{2} - 16.800T^{-1}$
$\Delta Gr° = 17.593 + 4.932 \times 10^{-3}T\ln T - 0.326 \times 10^{-6}T^{2} - 8.400T^{-1} - 36.611 \times 10^{-3}T$

1408-2000 K:
$\Delta Hr° = 18.900 - 7.412 \times 10^{-3}T + 0.326 \times 10^{-6}T^{2} - 16.800T^{-1}$
$\Delta Gr° = 18.900 + 7.412 \times 10^{-3}T\ln T - 0.326 \times 10^{-6}T^{2} - 8.400T^{-1} - 55.519 \times 10^{-3}T$

Source: Data are those estimated by Gronvold (187).

$U_3Si(c)$
Triuranium Silicide
[Formation: $3U(c) + Si(c) = U_3Si(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	25.790	41.590	41.590	0	-24.900	-25.225	18.490
300	25.820	41.750	41.590	.048	-24.897	-25.226	18.377
400	27.630	49.430	42.625	2.722	-24.788	-25.357	13.854
500	29.280	55.780	44.646	5.567	-24.697	-25.512	11.151
600	30.860	61.260	46.970	8.574	-24.653	-25.683	9.355
700	32.430	66.130	49.360	11.739	-24.683	-25.847	8.070
800	33.990	70.550	51.726	15.059	-24.827	-25.997	7.102
900	35.520	74.640	54.046	18.535	-25.118	-26.124	6.344
942	36.171	76.275	55.001	20.041	-25.294	-26.169	6.071
942	36.171	76.275	55.001	20.041	-27.295	-26.169	6.071
1000	37.070	78.470	56.306	22.164	-27.322	-26.098	5.704
1038	37.640	79.870	57.148	23.583	-27.312	-26.054	5.486
1038	37.310	80.810	57.148	24.563	-26.332	-26.054	5.486
1049	37.310	81.203	57.396	24.973	-26.330	-26.049	5.427
1049	37.310	81.203	57.396	24.973	-29.741	-26.049	5.427
1100	37.310	82.980	58.546	26.877	-29.564	-25.889	5.144
1200	37.310	86.230	60.723	30.609	-29.221	-25.574	4.658

Phase changes:
942 K, α − β transition point of U; ΔH° = 0.667 kcal/mol.
1038 K, δ − δ' transition point of U_3Si; ΔH° = 0.980 kcal/mol.
1049 K, β − γ transition point of U; ΔH° = 1.137 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1038 K: $Cp° = 21.865 + 15.252\times10^{-3}T - 0.555\times10^{5}T^{-2}$
$H°-H°_{298} = 21.865\times10^{-3}T + 7.626\times10^{-6}T^{2} + 0.555\times10^{2}T^{-1} - 7.383$
1038-1200 K: $Cp° = 37.318$
$H°-H°_{298} = 37.318\times10^{-3}T - 14.173$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf° = -27.201 + 6.856\times10^{-3}T - 5.391\times10^{-6}T^{2} + 219.500T^{-1}$
$\Delta Gf° = -27.201 - 6.856\times10^{-3}T\ln T + 5.391\times10^{-6}T^{2} + 109.750T^{-1} + 42.849\times10^{-3}T$
942-1038 K: $\Delta Hf° = -19.971 - 14.579\times10^{-3}T + 7.275\times10^{-6}T^{2} - 43.000T^{-1}$
$\Delta Gf° = -19.971 + 14.579\times10^{-3}T\ln T - 7.275\times10^{-6}T^{2} - 21.500T^{-1} - 99.534\times10^{-3}T$
1038-1049 K: $\Delta Hf° = -26.761 + 0.874\times10^{-3}T - 0.351\times10^{-6}T^{2} - 98.500T^{-1}$
$\Delta Gf° = -26.761 - 0.874\times10^{-3}T\ln T + 0.351\times10^{-6}T^{2} - 49.250T^{-1} + 6.439\times10^{-3}T$
1049-1200 K: $\Delta Hf° = -33.650 + 4.189\times10^{-3}T - 0.351\times10^{-6}T^{2} - 98.500T^{-1}$
$\Delta Gf° = -33.650 - 4.189\times10^{-3}T\ln T + 0.351\times10^{-6}T^{2} - 49.250T^{-1} + 36.064\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from O'Hare (363). Other data from Flotow (152).

UTe(g)
Uranium Monotelluride (ideal gas)
[Reaction: $U(c,l) + 0.5Te_2(g) = UTe(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	8.852	67.570	67.570	0	76.835	69.490	-50.937
300	8.855	67.625	67.572	.016	76.831	69.444	-50.589
400	9.040	70.197	67.920	.911	76.601	67.015	-36.615
500	9.232	72.235	68.585	1.825	76.330	64.650	-28.258
600	9.412	73.935	69.340	2.757	76.009	62.345	-22.709
700	9.568	75.398	70.104	3.706	75.626	60.097	-18.763
800	9.699	76.684	70.846	4.670	75.163	57.907	-15.819
900	9.806	77.833	71.561	5.645	74.609	55.782	-13.546
942	9.842	78.281	71.850	6.058	74.344	54.909	-12.739
942	9.842	78.281	71.850	6.058	73.677	54.909	-12.739
1000	9.892	78.871	72.241	6.630	73.370	53.762	-11.750
1049	9.925	79.345	72.562	7.116	73.111	52.808	-11.002
1049	9.925	79.345	72.562	7.116	71.974	52.808	-11.002
1100	9.959	79.817	72.887	7.623	71.760	51.883	-10.308
1200	10.008	80.686	73.501	8.622	71.340	50.096	-9.124
1300	10.042	81.488	74.085	9.624	70.914	48.342	-8.127
1400	10.062	82.233	74.641	10.629	70.483	46.622	-7.278
1408	10.063	82.290	74.684	10.709	70.449	46.486	-7.215
1408	10.063	82.290	74.684	10.709	68.264	46.486	-7.215
1500	10.071	82.928	75.171	11.636	67.640	45.081	-6.568
1600	10.071	83.578	75.676	12.643	66.962	43.596	-5.955
1700	10.062	84.188	76.159	13.650	66.285	42.164	-5.420
1800	10.047	84.763	76.621	14.656	65.608	40.761	-4.949
1900	10.027	85.305	77.063	15.659	64.931	39.401	-4.532
2000	10.004	85.819	77.489	16.661	64.255	38.075	-4.161

*Data estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.221 + 0.600\times10^{-3}T - 0.487\times10^{5}T^{-2}$
$H° - H°_{298} = 9.221\times10^{-3}T + 0.300\times10^{-6}T^{2} + 0.487\times10^{2}T^{-1} - 2.939$

Reaction equations (kcal/mol):

298.15-942 K: $ΔHr° = 76.254 + 1.811\times10^{-3}T - 4.218\times10^{-6}T^{2} + 124.100T^{-1}$
$ΔGr° = 76.254 - 1.811\times10^{-3}T\ln T + 4.218\times10^{-6}T^{2} + 62.050T^{-1} - 14.320\times10^{-3}T$
942-1049 K: $ΔHr° = 78.664 - 5.334\times10^{-3}T + 0.004\times10^{-6}T^{2} + 36.600T^{-1}$
$ΔGr° = 78.664 + 5.334\times10^{-3}T\ln T - 0.004\times10^{-6}T^{2} + 18.300T^{-1} - 61.781\times10^{-3}T$
1049-1408 K: $ΔHr° = 76.368 - 4.228\times10^{-3}T + 0.004\times10^{-6}T^{2} + 36.600T^{-1}$
$ΔGr° = 76.368 + 4.228\times10^{-3}T\ln T - 0.004\times10^{-6}T^{2} + 18.300T^{-1} - 51.906\times10^{-3}T$
1408-2000 K: $ΔHr° = 77.674 - 6.709\times10^{-3}T + 0.004\times10^{-6}T^{2} + 36.600T^{-1}$
$ΔGr° = 77.674 + 6.709\times10^{-3}T\ln T - 0.004\times10^{-6}T^{2} + 18.300T^{-1} - 70.814\times10^{-3}T$

Source: Data are those estimated by Gronvold (187).

$UTe_2(g)$
Uranium Ditelluride (ideal gas)
[Reaction: $U(c,l) + Te_2(g) = UTe_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	14.567	78.030	78.030	0	32.670	31.430	-23.038
300	14.571	78.120	78.030	.027	32.669	31.421	-22.890
400	14.713	82.333	78.603	1.492	32.569	31.019	-16.948
500	14.781	85.624	79.690	2.967	32.412	30.650	-13.397
600	14.818	88.323	80.911	4.447	32.182	30.321	-11.044
700	14.841	90.609	82.138	5.930	31.868	30.034	-9.377
800	14.855	92.591	83.322	7.415	31.454	29.796	-8.140
900	14.865	94.342	84.452	8.901	30.930	29.618	-7.192
942	14.868	95.020	84.908	9.525	30.673	29.562	-6.858
942	14.868	95.020	84.908	9.525	30.006	29.562	-6.858
1000	14.873	95.908	85.520	10.388	29.704	29.544	-6.457
1049	14.875	96.620	86.022	11.117	29.446	29.543	-6.155
1049	14.875	96.620	86.022	11.117	28.309	29.543	-6.155
1100	14.878	97.326	86.531	11.875	28.092	29.611	-5.883
1200	14.882	98.621	87.485	13.363	27.655	29.769	-5.422
1300	14.885	99.812	88.387	14.852	27.204	29.964	-5.037
1400	14.888	100.915	89.244	16.340	26.736	30.193	-4.713
1408	14.888	101.000	89.310	16.459	26.698	30.213	-4.690
1408	14.888	101.000	89.310	16.459	24.513	30.213	-4.690
1500	14.890	101.942	90.056	17.829	23.852	30.605	-4.459
1600	14.892	102.903	90.829	19.318	23.134	31.072	-4.244
1700	14.893	103.806	91.567	20.807	22.418	31.603	-4.063
1800	14.894	104.658	92.271	22.297	21.706	32.157	-3.904
1900	14.895	105.463	92.944	23.786	20.997	32.758	-3.768
2000	14.896	106.227	93.589	25.276	20.294	33.398	-3.650

*Data estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.896 + 0.004\times10^{-3}T - 0.294\times10^{5}T^{-2}$
$H°-H°_{298} = 14.896\times10^{-3}T + 0.002\times10^{-6}T^{2} + 0.294\times10^{2}T^{-1} - 4.540$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta Hr° = 31.837 + 3.187\times10^{-3}T - 4.813\times10^{-6}T^{2} + 92.700T^{-1}$
$\Delta Gr° = 31.837 - 3.187\times10^{-3}T\ln T + 4.813\times10^{-6}T^{2} + 46.350T^{-1} + 14.837\times10^{-3}T$
942-1049 K: $\Delta Hr° = 34.247 - 3.958\times10^{-3}T - 0.591\times10^{-6}T^{2} + 5.200T^{-1}$
$\Delta Gr° = 34.247 + 3.958\times10^{-3}T\ln T + 0.591\times10^{-6}T^{2} + 2.600T^{-1} - 32.624\times10^{-3}T$
1049-1408 K: $\Delta Hr° = 31.951 - 2.853\times10^{-3}T - 0.591\times10^{-6}T^{2} + 5.200T^{-1}$
$\Delta Gr° = 31.951 + 2.853\times10^{-3}T\ln T + 0.591\times10^{-6}T^{2} + 2.600T^{-1} - 22.750\times10^{-3}T$
1408-2000 K: $\Delta Hr° = 33.257 - 5.333\times10^{-3}T - 0.591\times10^{-6}T^{2} + 5.200T^{-1}$
$\Delta Gr° = 33.257 + 5.333\times10^{-3}T\ln T + 0.591\times10^{-6}T^{2} + 2.600T^{-1} - 41.657\times10^{-3}T$

Source: Data are those estimated by Gronvold (187).

VB(c)
Vanadium Boride
[Formation: V(c,l) + B(β,l) = VB(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.609	7.000	7.000	0	-33.100	-32.705	23.973
300	8.642	7.053	7.000	.016	-33.100	-32.701	23.823
400	9.967	9.739	7.357	.953	-33.093	-32.571	17.796
500	10.815	12.060	8.072	1.994	-33.095	-32.439	14.179
600	11.464	14.091	8.909	3.109	-33.105	-32.309	11.769
700	12.008	15.900	9.780	4.284	-33.112	-32.175	10.045
800	12.488	17.535	10.649	5.509	-33.110	-32.040	8.753
900	12.922	19.032	11.499	6.780	-33.101	-31.906	7.748
1000	13.321	20.414	12.322	8.092	-33.088	-31.774	6.944
1100	13.689	21.701	13.116	9.443	-33.069	-31.649	6.288
1200	14.031	22.907	13.883	10.829	-33.051	-31.519	5.740
1300	14.483	24.049	14.621	12.256	-33.029	-31.388	5.277
1400	14.924	25.138	15.334	13.726	-33.002	-31.263	4.880
1500	15.384	26.184	16.023	15.241	-32.970	-31.137	4.537
1600	15.866	27.192	16.690	16.804	-32.930	-31.029	4.238
1700	16.367	28.168	17.336	18.415	-32.882	-30.910	3.974
1800	16.888	29.119	17.965	20.078	-32.823	-30.784	3.738
1900	17.430	30.046	18.576	21.793	-32.757	-30.671	3.528
2000	17.992	30.954	19.172	23.564	-32.681	-30.575	3.341
2100	18.575	31.846	19.754	25.393	-32.596	-30.460	3.170
2190	19.118	32.637	20.268	27.089	-32.517	-30.383	3.032
2190	19.118	32.637	20.268	27.089	-37.978	-30.383	3.032
2200	19.178	32.724	20.324	27.280	-37.973	-30.348	3.015
2300	19.801	33.590	20.882	29.229	-37.904	-29.990	2.850
2350	20.123	34.020	21.157	30.227	-37.851	-29.837	2.775
2350	20.123	34.020	21.157	30.227	-49.851	-29.837	2.775
2400	20.445	34.447	21.430	31.241	-49.764	-29.402	2.677
2500	21.109	35.295	21.967	33.319	-49.540	-28.572	2.498

Phase changes: 2190 K, melting point of V; ΔH° = 5.461 kcal/mol.
2350 K, melting point of B; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 9.175 + 4.362\times10^{-3}T - 1.660\times10^{5}T^{-2}$
$H°-H°_{298} = 9.175\times10^{-3}T + 2.181\times10^{-6}T^{2} + 1.660\times10^{2}T^{-1} - 3.486$

Formation equations (kcal/mol):

298.15-2190 K: $\Delta Hf° = -32.804 - 0.659\times10^{-3}T + 0.377\times10^{-6}T^{2} - 39.800T^{-1}$
$\Delta Gf° = -32.804 + 0.659\times10^{-3}T\ln T - 0.377\times10^{-6}T^{2} - 19.900T^{-1} - 3.088\times10^{-3}T$
2190-2350 K: $\Delta Hf° = -30.600 - 6.591\times10^{-3}T + 1.489\times10^{-6}T^{2} - 55.500T^{-1}$
$\Delta Gf° = -30.600 + 6.591\times10^{-3}T\ln T - 1.489\times10^{-6}T^{2} - 27.750T^{-1} - 47.284\times10^{-3}T$
2350-2500 K: $\Delta Hf° = -39.989 - 9.368\times10^{-3}T + 2.181\times10^{-6}T^{2} + 166.000T^{-1}$
$\Delta Gf° = -39.989 + 9.368\times10^{-3}T\ln T - 2.181\times10^{-6}T^{2} + 83.000T^{-1} - 63.238\times10^{-3}T$

Source: Data from Barin (23).

$VB_2(c)$
Vanadiun Diboride
[Formation: $V(c,l) + 2B(\beta,l) = VB_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.229	7.200	7.200	0	-48.700	-47.944	35.144
300	11.290	7.270	7.200	.021	-48.700	-47.937	34.922
400	13.721	10.884	7.676	1.283	-48.685	-47.689	26.056
500	15.248	14.120	8.648	2.736	-48.682	-47.436	20.734
600	16.382	17.005	9.805	4.320	-48.698	-47.191	17.189
700	17.301	19.601	11.022	6.005	-48.713	-46.936	14.654
800	18.076	21.963	12.244	7.775	-48.712	-46.680	12.752
900	18.744	24.132	13.446	9.617	-48.701	-46.426	11.274
1000	19.323	26.138	14.617	11.521	-48.684	-46.174	10.091
1100	19.823	28.003	15.749	13.479	-48.662	-45.935	9.126
1200	20.282	29.747	16.844	15.483	-48.645	-45.685	8.320
1300	20.878	31.395	17.900	17.543	-48.624	-45.431	7.638
1400	21.464	32.964	18.921	19.660	-48.598	-45.188	7.054
1500	22.069	34.465	19.908	21.836	-48.568	-44.936	6.547
1600	22.696	35.909	20.880	24.047	-48.558	-44.748	6.112
1700	23.342	37.304	21.789	26.376	-48.484	-44.482	5.719
1800	24.008	38.657	22.689	28.743	-48.427	-44.224	5.369
1900	24.695	39.974	23.565	31.178	-48.361	-43.991	5.060
2000	25.402	41.258	24.417	33.683	-48.285	-43.787	4.785
2100	26.130	42.515	25.249	36.259	-48.201	-43.543	4.532
2190	26.803	43.626	25.981	38.642	-48.120	-43.367	4.328
2190	26.803	43.626	25.981	38.642	-53.581	-43.367	4.328
2200	26.878	43.748	26.062	38.910	-53.576	-43.320	4.303
2300	27.646	44.960	26.857	41.636	-53.506	-42.832	4.070
2350	28.041	45.558	27.249	43.027	-53.453	-42.635	3.965
2350	28.041	45.558	27.249	43.027	-77.453	-42.635	3.965
2400	28.435	46.153	27.637	44.439	-77.343	-41.876	3.813
2500	29.244	47.330	28.401	47.323	-77.063	-40.433	3.535

Phase changes: 2190 K, melting point of V; ΔH° = 5.461 kcal/mol.
2350 K, melting point of B; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 13.884 + 5.760\times10^{-3}T - 3.886\times10^{5}T^{-2}$
$H°- H°_{298} = 13.884\times10^{-3}T + 2.880\times10^{-6}T^{2} + 3.886\times10^{2}T^{-1} - 5.699$

Formation equations (kcal/mol):

298.15-2190 K: $\Delta Hf° = -48.404 - 0.673\times10^{-3}T + 0.384\times10^{-6}T^{2} - 38.700T^{-1}$
$\Delta Gf° = -48.404 + 0.673\times10^{-3}T\ln T - 0.384\times10^{-6}T^{2} - 19.350T^{-1} - 1.961\times10^{-3}T$
2190-2350 K: $\Delta Hf° = -46.200 - 6.605\times10^{-3}T + 1.496\times10^{-6}T^{2} - 54.400T^{-1}$
$\Delta Gf° = -46.200 + 6.605\times10^{-3}T\ln T - 1.496\times10^{-6}T^{2} - 27.200T^{-1} - 46.158\times10^{-3}T$
2350-2500 K: $\Delta Hf° = -64.979 - 12.159\times10^{-3}T + 2.880\times10^{-6}T^{2} + 388.600T^{-1}$
$\Delta Gf° = -64.979 + 12.159\times10^{-3}T\ln T - 2.880\times10^{-6}T^{2} + 194.300T^{-1} - 78.065\times10^{-3}T$

Source: Data from Barin (23).

$V_2B_3(c)$
Divanadium Triboride
[Formation: $2V(c,l) + 3B(\beta,l) = V_2B_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.837	14.200	14.200	0	-82.500	-81.349	59.630
300	19.931	14.323	14.200	.037	-82.500	-81.339	59.254
400	23.688	20.623	15.033	2.236	-82.478	-80.961	44.234
500	26.063	26.180	16.720	4.730	-82.477	-80.576	35.219
600	27.847	31.095	18.713	7.429	-82.503	-80.200	29.212
700	29.310	35.501	20.802	10.289	-82.525	-79.811	24.918
800	30.565	39.499	22.894	13.284	-82.522	-79.420	21.696
900	31.668	43.164	24.945	16.397	-82.502	-79.032	19.191
1000	32.645	46.552	26.938	19.614	-82.471	-78.647	17.188
1100	33.513	49.705	28.867	22.922	-82.431	-78.285	15.554
1200	34.283	52.654	30.726	26.313	-82.395	-77.902	14.188
1300	35.361	55.444	32.522	29.799	-82.353	-77.520	13.032
1400	36.388	58.102	34.255	33.386	-82.300	-77.151	12.044
1500	37.455	60.649	35.930	37.078	-82.237	-76.772	11.186
1600	38.563	63.101	37.552	40.879	-82.160	-76.450	10.442
1700	39.710	65.473	39.125	44.792	-82.065	-76.093	9.782
1800	40.898	67.776	40.653	48.822	-81.949	-75.707	9.192
1900	42.127	70.020	42.139	52.973	-81.816	-75.360	8.668
2000	43.397	72.213	43.588	57.249	-81.664	-75.062	8.202
2100	44.707	74.362	45.003	61.654	-81.495	-74.704	7.774
2190	45.923	76.263	46.249	65.732	-81.334	-74.449	7.430
2190	45.923	76.263	46.249	65.732	-92.256	-74.449	7.430
2200	46.058	76.473	46.386	66.192	-92.247	-74.368	7.388
2300	47.450	78.551	47.739	70.867	-92.108	-73.522	6.986
2350	48.166	79.579	48.406	73.257	-92.001	-73.171	6.805
2350	48.166	79.579	48.406	73.257	-128.001	-73.171	6.805
2400	48.882	80.601	49.066	75.683	-127.804	-71.978	6.554
2500	50.355	82.626	50.368	80.645	-127.300	-69.705	6.094

Phase changes: 2190 K, melting point of V; ΔH° = 5.461 kcal/mol.
2350 K, melting point of B; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 22.955 + 10.194\times10^{-3}T - 5.474\times10^{5}T^{-2}$

$H°- H°_{298} = 22.955\times10^{-3}T + 5.097\times10^{-6}T^{2} + 5.474\times10^{2}T^{-1} - 9.133$

Formation equations (kcal/mol):

298.15-2190 K: $\Delta Hf° = -81.855 - 1.436\times10^{-3}T + 0.797\times10^{-6}T^{2} - 85.700T^{-1}$

$\Delta Gf° = -81.855 + 1.436\times10^{-3}T\ln T - 0.797\times10^{-6}T^{2} - 42.850T^{-1} - 5.765\times10^{-3}T$

2190-2350 K: $\Delta Hf° = -77.447 - 13.300\times10^{-3}T + 3.021\times10^{-6}T^{2} - 117.100T^{-1}$

$\Delta Gf° = -77.447 + 13.300\times10^{-3}T\ln T - 3.021\times10^{-6}T^{2} - 58.550T^{-1} - 94.157\times10^{-3}T$

2350-2500 K: $\Delta Hf° = -105.617 - 21.631\times10^{-3}T + 5.097\times10^{-6}T^{2} + 547.400T^{-1}$

$\Delta Gf° = -105.617 + 21.631\times10^{-3}T\ln T - 5.097\times10^{-6}T^{2} + 273.700T^{-1} - 142.018\times10^{-3}T$

Source: Data from Barin (23).

V_3B_2(c)
Trivanadium Diboride
[Formation: $3V(c,l) + 2B(\beta,l) = V_3B_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.207	20.780	20.780	0	-72.600	-71.770	52.608
300	23.278	20.924	20.781	.043	-72.600	-71.762	52.278
400	26.148	28.052	21.732	2.528	-72.588	-71.489	39.059
500	28.014	34.098	23.616	5.241	-72.597	-71.209	31.125
600	29.475	39.339	25.811	8.117	-72.621	-70.934	25.837
700	30.734	43.979	28.080	11.129	-72.637	-70.650	22.058
800	31.877	48.158	30.333	14.260	-72.629	-70.364	19.222
900	32.945	51.975	32.528	17.502	-72.604	-70.080	17.017
1000	33.961	55.499	34.652	20.847	-72.568	-69.803	15.255
1100	34.935	58.782	36.697	24.293	-72.514	-69.540	13.816
1200	35.875	61.862	38.668	27.833	-72.459	-69.267	12.615
1300	37.054	64.782	40.565	31.482	-72.391	-68.997	11.599
1400	38.232	67.571	42.395	35.246	-72.308	-68.739	10.731
1500	39.470	70.251	44.164	39.131	-72.209	-68.478	9.977
1600	40.768	72.839	45.875	43.142	-72.089	-68.263	9.324
1700	42.127	75.351	47.536	47.286	-71.942	-68.027	8.745
1800	43.547	77.799	49.150	51.569	-71.765	-67.774	8.229
1900	45.027	80.193	50.721	55.997	-71.564	-67.557	7.771
2000	46.569	82.541	52.253	60.577	-71.335	-67.375	7.362
2100	48.172	84.852	53.751	65.313	-71.083	-67.162	6.990
2190	49.670	86.904	55.071	69.715	-70.844	-67.024	6.689
2190	49.670	86.904	55.071	69.715	-87.227	-67.024	6.689
2200	49.836	87.131	55.216	70.213	-87.213	-66.931	6.649
2300	51.561	89.384	56.653	75.282	-87.008	-65.988	6.270
2350	52.454	90.502	57.361	77.882	-86.850	-65.566	6.098
2350	52.454	90.502	57.361	77.882	-110.850	-65.566	6.098
2400	53.347	91.616	58.063	80.527	-110.611	-64.586	5.881
2500	55.194	93.831	59.449	85.954	-109.996	-62.708	5.482

Phase changes: 2190 K, melting point of V; ΔH° = 5.461 kcal/mol.
2350 K, melting point of B; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 22.716 + 11.764\times10^{-3}T - 2.681\times10^{5}T^{-2}$
$H°- H°_{298} = 22.716\times10^{-3}T + 5.882\times10^{-6}T^{2} + 2.681\times10^{2}T^{-1} - 8.195$

Formation equations (kcal/mol):

298.15-2190 K: $\Delta Hf° = -71.660 - 2.063\times10^{-3}T + 1.162\times10^{-6}T^{2} - 127.800T^{-1}$
$\Delta Gf° = -71.660 + 2.063\times10^{-3}T\ln T - 1.162\times10^{-6}T^{2} - 63.900T^{-1} - 11.058\times10^{-3}T$
2190-2350 K: $\Delta Hf° = -65.048 - 19.859\times10^{-3}T + 4.498\times10^{-6}T^{2} - 174.900T^{-1}$
$\Delta Gf° = -65.048 + 19.859\times10^{-3}T\ln T - 4.498\times10^{-6}T^{2} - 87.450T^{-1} - 143.647\times10^{-3}T$
2350-2500 K: $\Delta Hf° = -83.827 - 25.413\times10^{-3}T + 5.882\times10^{-6}T^{2} + 268.100T^{-1}$
$\Delta Gf° = -83.827 + 25.413\times10^{-3}T\ln T - 5.882\times10^{-6}T^{2} + 134.050T^{-1} - 175.555\times10^{-3}T$

Source: Data from Barin (23).

$V_3B_4(c)$
Trivanadium Tetraboride
[Formation: $3V(c,l) + 4B(\beta,l) = V_3B_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	28.445	21.190	21.190	0	-116.300	-114.751	84.114
300	28.572	21.366	21.190	.053	-116.300	-114.737	83.585
400	33.655	30.352	22.382	3.188	-116.272	-114.229	62.411
500	36.878	38.229	24.781	6.724	-116.272	-113.710	49.702
600	39.311	45.176	27.613	10.538	-116.308	-113.203	41.234
700	41.319	51.391	30.572	14.573	-116.337	-112.679	35.179
800	43.054	57.024	33.533	18.793	-116.332	-112.152	30.638
900	44.591	62.185	36.433	23.177	-116.303	-111.627	27.107
1000	45.966	66.956	39.250	27.706	-116.259	-111.111	24.283
1100	47.204	71.396	41.973	32.365	-116.200	-110.623	21.978
1200	48.315	75.552	44.600	37.142	-116.146	-110.110	20.054
1300	49.844	79.484	47.133	42.056	-116.081	-109.595	18.424
1400	51.312	83.231	49.579	47.113	-116.001	-109.100	17.031
1500	52.840	86.823	51.943	52.320	-115.906	-108.593	15.822
1600	54.428	90.281	54.229	57.683	-115.790	-108.160	14.774
1700	56.077	93.632	56.451	63.208	-115.646	-107.687	13.844
1800	57.787	96.886	58.608	68.900	-115.472	-107.174	13.013
1900	59.557	100.057	60.706	74.767	-115.272	-106.712	12.275
2000	61.389	103.159	62.752	80.814	-115.044	-106.320	11.618
2100	63.282	106.199	64.748	87.047	-114.791	-105.845	11.015
2190	65.041	108.891	66.508	92.819	-114.553	-105.514	10.530
2190	65.041	108.891	66.508	92.819	-130.936	-105.514	10.530
2200	65.236	109.188	66.702	93.470	-130.922	-105.398	10.470
2300	67.251	112.132	68.612	100.096	-130.712	-104.191	9.900
2350	68.289	113.589	69.554	103.484	-130.552	-103.683	9.642
2350	68.289	113.589	69.554	103.484	-178.552	-103.683	9.642
2400	69.327	115.038	70.486	106.924	-178.268	-102.056	9.293
2500	71.464	117.911	72.326	113.963	-177.541	-98.954	8.650

Phase changes: 2190 K, melting point of V; ΔH° = 5.461 kcal/mol.
2350 K, melting point of B; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 32.340 + 14.412\times10^{-3}T - 7.283\times10^{5}T^{-2}$
$H°-H°_{298} = 32.340\times10^{-3}T + 7.206\times10^{-6}T^{2} + 7.283\times10^{2}T^{-1} - 12.725$

Formation equations (kcal/mol):

298.15-2190 K: $\Delta Hf° = -115.465 - 1.885\times10^{-3}T + 1.102\times10^{-6}T^{2} - 110.600T^{-1}$
$\Delta Gf° = -115.465 + 1.885\times10^{-3}T\ln T - 1.102\times10^{-6}T^{2} - 55.300T^{-1} - 7.395\times10^{-3}T$
2190-2350 K: $\Delta Hf° = -108.853 - 19.681\times10^{-3}T + 4.438\times10^{-6}T^{2} - 157.700T^{-1}$
$\Delta Gf° = -108.853 + 19.681\times10^{-3}T\ln T - 4.438\times10^{-6}T^{2} - 78.850T^{-1} - 139.984\times10^{-3}T$
2350-2500 K: $\Delta Hf° = -146.413 - 30.789\times10^{-3}T + 7.206\times10^{-6}T^{2} + 728.300T^{-1}$
$\Delta Gf° = -146.413 + 30.789\times10^{-3}T\ln T - 7.206\times10^{-6}T^{2} + 364.150T^{-1} - 203.799\times10^{-3}T$

Source: Data from Barin (23).

V_5B_6(c)
Pentavanadium Hexaboride
[Formation: $5V(c,l) + 6B(\beta,l) = V_5B_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	45.663	18.200	18.200	0	-182.500	-175.095	128.347
300	45.857	18.483	18.200	.085	-182.500	-175.043	127.517
400	53.590	32.840	20.105	5.094	-182.458	-172.576	94.290
500	58.509	45.358	23.932	10.713	-182.461	-170.092	74.346
600	62.240	56.368	28.440	16.757	-182.517	-167.627	61.057
700	65.336	66.201	33.144	23.140	-182.562	-165.136	51.557
800	68.031	75.105	37.841	29.811	-182.552	-162.640	44.431
900	70.436	83.259	42.441	36.736	-182.506	-160.149	38.889
1000	72.609	90.795	46.905	43.890	-182.435	-157.670	34.458
1100	74.583	97.809	51.217	51.251	-182.338	-155.233	30.842
1200	76.379	104.377	55.376	58.801	-182.247	-152.759	27.821
1300	78.812	110.593	59.386	66.569	-182.138	-150.285	25.265
1400	81.161	116.519	63.257	74.567	-182.003	-147.842	23.079
1500	83.611	122.202	66.999	82.804	-181.844	-145.382	21.182
1600	86.162	127.679	70.622	91.292	-181.649	-143.039	19.538
1700	88.814	132.981	74.134	100.040	-181.408	-140.627	18.079
1800	91.567	138.135	77.547	109.058	-181.116	-138.159	16.775
1900	94.421	143.162	80.869	118.357	-180.782	-135.775	15.617
2000	97.378	148.080	84.107	127.946	-180.402	-133.492	14.587
2100	100.436	152.905	87.269	137.836	-179.980	-131.092	13.643
2190	103.280	157.178	90.054	147.002	-179.580	-129.072	12.881
2190	103.280	157.178	90.054	147.002	-206.885	-129.072	12.881
2200	103.596	157.649	90.360	148.036	-206.862	-128.716	12.787
2300	106.857	162.326	93.388	158.558	-206.516	-125.098	11.887
2350	108.539	164.642	94.880	163.942	-206.249	-123.433	11.479
2350	108.539	164.642	94.880	163.942	-278.249	-123.433	11.479
2400	110.221	166.945	96.357	169.411	-277.791	-120.087	10.935
2500	113.687	171.514	99.272	180.606	-276.616	-113.626	9.933

Phase changes: 2190 K, melting point of V; ΔH° = 5.461 kcal/mol.
2350 K, melting point of B; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 50.690 + 23.140\text{x}10^{-3}T - 10.602\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 50.690\text{x}10^{-3}T + 11.570\text{x}10^{-6}T^{2} + 10.602\text{x}10^{2}T^{-1} - 19.698$

Formation equations (kcal/mol):

298.15-2190 K: $\Delta Hf° = -181.072 - 3.203\text{x}10^{-3}T + 1.858\text{x}10^{-6}T^{2} - 190.300T^{-1}$
$\Delta Gf° = -181.072 + 3.203\text{x}10^{-3}T\ln T - 1.858\text{x}10^{-6}T^{2} - 95.150T^{-1} + 3.420\text{x}10^{-3}T$
2190-2350 K: $\Delta Hf° = -170.052 - 32.863\text{x}10^{-3}T + 7.418\text{x}10^{-6}T^{2} - 268.800T^{-1}$
$\Delta Gf° = -170.052 + 32.863\text{x}10^{-3}T\ln T - 7.418\text{x}10^{-6}T^{2} - 134.400T^{-1} - 217.562\text{x}10^{-3}T$
2350-2500 K: $\Delta Hf° = -226.391 - 49.525\text{x}10^{-3}T + 11.570\text{x}10^{-6}T^{2} + 1060.200T^{-1}$
$\Delta Gf° = -226.391 + 49.525\text{x}10^{-3}T\ln T - 11.570\text{x}10^{-6}T^{2} + 530.100T^{-1} - 313.284\text{x}10^{-3}T$

Source: Data from Barin (23).

$VC_{0.5}(c)$
Vanadium Carbide
[Formation: $V(c) + 0.5C(c) = VC_{0.5}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	6.680	6.110	6.110	0	-14.000	-13.555	9.936
300	6.700	6.150	6.117	.010	-14.003	-13.555	9.874
400	7.660	8.220	6.395	.730	-14.018	-13.404	7.324
500	8.330	10.000	6.920	1.540	-14.003	-13.240	5.787
600	8.840	11.570	7.570	2.400	-13.981	-13.091	4.768
700	9.260	12.970	8.256	3.300	-13.957	-12.955	4.045
800	9.620	14.230	8.930	4.240	-13.924	-12.817	3.502
900	9.930	15.380	9.580	5.220	-13.880	-12.678	3.079
1000	10.210	16.440	10.210	6.230	-13.835	-12.544	2.741
1100	10.460	17.420	10.820	7.260	-13.795	-12.410	2.466
1200	10.700	18.340	11.407	8.320	-13.753	-12.288	2.238
1300	10.920	19.210	11.979	9.400	-13.719	-12.175	2.047
1400	11.140	20.030	12.523	10.510	-13.683	-12.054	1.882
1500	11.340	20.800	13.047	11.630	-13.667	-11.934	1.739
1600	11.540	21.540	13.559	12.770	-13.659	-11.827	1.615
1700	11.730	22.250	14.050	13.940	-13.651	-11.715	1.506
1800	11.920	22.920	14.520	15.120	-13.663	-11.591	1.407

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 7.832 + 2.444 \times 10^{-3}T - 1.672 \times 10^{5}T^{-2}$

$H° - H°_{298} = 7.832 \times 10^{-3}T + 1.222 \times 10^{-6}T^{2} + 1.672 \times 10^{2}T^{-1} - 3.005$

Formation equations (kcal/mol):

298.15-1800 K: $\Delta Hf° = -14.587 + 0.962 \times 10^{-3}T - 0.273 \times 10^{-6}T^{2} + 96.750T^{-1}$

$\Delta Gf° = -14.587 - 0.962 \times 10^{-3}T\ln T + 0.273 \times 10^{-6}T^{2} + 48.375T^{-1} + 8.315 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Storms (477) and Pillai (402). Low-temperature heat capacities from Chernyaev (87). High-temperature data based on Chernyaev (86).

$VC_{0.88}$(c)
Vanadium Carbide
[Formation: $V(c,l) + 0.88C(c) = VC_{0.88}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	7.640	6.000	6.000	0	-24.300	-23.667	17.348
300	7.680	6.047	6.014	.010	-24.305	-23.667	17.241
400	9.340	8.512	6.312	.880	-24.262	-23.449	12.812
500	10.280	10.705	6.985	1.860	-24.197	-23.258	10.166
600	10.940	12.641	7.774	2.920	-24.119	-23.079	8.406
700	11.450	14.367	8.596	4.040	-24.036	-22.914	7.154
800	11.880	15.924	9.411	5.210	-23.947	-22.756	6.216
900	12.250	17.345	10.212	6.420	-23.859	-22.609	5.490
1000	12.580	18.652	10.992	7.660	-23.776	-22.476	4.912
1100	12.880	19.865	11.747	8.930	-23.695	-22.343	4.439
1200	13.150	20.998	12.473	10.230	-23.617	-22.236	4.050
1300	13.400	22.061	13.169	11.560	-23.542	-22.122	3.719
1400	13.640	23.063	13.842	12.910	-23.479	-22.018	3.437
1500	13.850	24.011	14.484	14.290	-23.419	-21.909	3.192
1600	14.040	24.911	15.111	15.680	-23.379	-21.815	2.980
1700	14.220	25.767	15.714	17.090	-23.352	-21.722	2.792
1800	14.380	26.585	16.296	18.520	-23.337	-21.625	2.626
1900	14.520	27.366	16.855	19.970	-23.337	-21.525	2.476
2000	14.650	28.114	17.399	21.430	-23.364	-21.427	2.341
2100	14.760	28.831	17.926	22.900	-23.420	-21.329	2.220
2190	14.841	29.452	18.388	24.232	-23.499	-21.241	2.120
2190	14.841	29.452	18.388	24.232	-28.960	-21.241	2.120
2200	14.850	29.520	18.438	24.380	-28.975	-21.206	2.107
2300	14.930	30.182	18.934	25.870	-29.126	-20.846	1.981
2400	15.000	30.819	19.419	27.360	-29.281	-20.491	1.866
2500	15.050	31.433	19.885	28.870	-29.418	-20.115	1.758

Phase change: 2190 K, melting point of V; ΔH° = 5.461 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 10.835 + 1.966\times10^{-3}T - 3.361\times10^{5}T^{-2}$
$H°-H°_{298} = 10.835\times10^{-3}T + 0.983\times10^{-6}T^{2} + 3.361\times10^{2}T^{-1} - 4.445$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -25.684 + 2.628\times10^{-3}T - 0.803\times10^{-6}T^{2} + 200.176T^{-1}$
$\Delta Gf° = -25.684 - 2.628\times10^{-3}T\ln T + 0.803\times10^{-6}T^{2} + 100.088T^{-1} + 20.372\times10^{-3}T$
2000-2190 K: $\Delta Hf° = -23.931 + 0.760\times10^{-3}T - 0.247\times10^{-6}T^{2} - 281.800T^{-1}$
$\Delta Gf° = -23.931 - 0.760\times10^{-3}T\ln T + 0.247\times10^{-6}T^{2} - 140.900T^{-1} + 6.468\times10^{-3}T$
2190-2500 K: $\Delta Hf° = -21.727 - 5.172\times10^{-3}T + 0.865\times10^{-6}T^{2} - 297.500T^{-1}$
$\Delta Gf° = -21.727 + 5.172\times10^{-3}T\ln T - 0.865\times10^{-6}T^{2} - 148.750T^{-1} - 37.729\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Low-temperature heat capacities and entropy at 298 K from Chernyaev (87). High-temperature data based on Chernyaev (86), Volokova (511), and Turchanin (506).

$VN_{0.465}(c)$
Vanadium Subnitride
[Formation: $V(c) + 0.2325N_2(g) = VN_{0.465}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	6.902	6.379	6.379	0	-31.800	-28.467	20.867
300	6.924	6.422	6.379	.013	-31.801	-28.447	20.723
400	7.810	8.549	6.661	.755	-31.834	-27.321	14.928
500	8.431	10.362	7.226	1.568	-31.821	-26.195	11.450
600	8.898	11.942	7.882	2.436	-31.768	-25.073	9.133
700	9.264	13.342	8.565	3.344	-31.693	-23.964	7.482
800	9.570	14.599	9.240	4.287	-31.600	-22.864	6.246
900	9.845	15.743	9.902	5.257	-31.500	-21.779	5.289
1000	10.107	16.794	10.539	6.255	-31.393	-20.706	4.525
1100	10.368	17.769	11.152	7.279	-31.280	-19.641	3.902
1200	10.630	18.682	11.741	8.329	-31.165	-18.587	3.385
1300	10.894	19.544	12.309	9.405	-31.048	-17.545	2.949
1400	11.154	20.361	12.856	10.507	-30.932	-16.511	2.577
1500	11.402	21.139	13.382	11.635	-30.817	-15.484	2.256
1600	11.629	21.882	13.890	12.787	-30.704	-14.467	1.976
1700	11.827	22.593	14.381	13.960	-30.598	-13.455	1.730
1800	11.991	23.274	14.857	15.151	-30.503	-12.449	1.511

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp^\circ = 7.776 + 2.468\text{x}10^{-3}T - 1.430\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.776\text{x}10^{-3}T + 1.234\text{x}10^{-6}T^{2} + 1.430\text{x}10^{2}T^{-1} - 2.908$

Formation equations (kcal/mol):

298.15-1800 K: $\Delta Hf^\circ = -32.680 + 1.150\text{x}10^{-3}T - 0.015\text{x}10^{-6}T^{2} + 160.537T^{-1}$

$\Delta Gf^\circ = -32.680 - 1.150\text{x}10^{-3}T\ln T + 0.015\text{x}10^{-6}T^{2} + 80.268T^{-1} + 19.772\text{x}10^{-3}T$

Source: Data from Pankratz (389).

VN(c)
Vanadium Nitride
[Formation: $V(c) + 0.5N_2(g) = VN(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	9.080	8.910	8.910	0	-51.880	-45.652	33.463
300	9.100	8.966	8.910	.017	-51.881	-45.613	33.228
400	10.280	11.796	9.288	1.003	-51.856	-43.526	23.781
500	10.990	14.170	10.034	2.068	-51.778	-41.451	18.118
600	11.550	16.225	10.898	3.196	-51.657	-39.396	14.350
700	12.000	18.040	11.791	4.374	-51.507	-37.365	11.666
800	12.350	19.666	12.676	5.592	-51.337	-35.356	9.659
900	12.640	21.138	13.536	6.842	-51.160	-33.368	8.103
1000	12.890	22.483	14.365	8.118	-50.982	-31.403	6.863
1100	13.100	23.721	15.159	9.418	-50.804	-29.452	5.852
1200	13.280	24.868	15.920	10.737	-50.634	-27.518	5.012
1300	13.450	25.938	16.650	12.074	-50.473	-25.597	4.303
1400	13.600	26.941	17.351	13.426	-50.327	-23.691	3.698
1500	13.740	27.884	18.022	14.793	-50.195	-21.793	3.175
1600	13.840	28.774	18.667	16.172	-50.079	-19.906	2.719

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp° = 10.987 + 2.026\text{x}10^{-3}T - 2.232\text{x}10^{5}T^{-2}$

$H° - H°_{298} = 10.987\text{x}10^{-3}T + 1.013\text{x}10^{-6}T^{2} + 2.232\text{x}10^{2}T^{-1} - 4.114$

Formation equations (kcal/mol):

298.15-1600 K: $\Delta Hf° = -53.440 + 2.618\text{x}10^{-3}T - 0.394\text{x}10^{-6}T^{2} + 242.850T^{-1}$

$\Delta Gf° = -53.440 - 2.618\text{x}10^{-3}T\ln T + 0.394\text{x}10^{-6}T^{2} + 121.425T^{-1} + 39.552\text{x}10^{-3}T$

Source: Data from Pankratz (389).

VN(g)
Vanadium Nitride (ideal gas)
[Formation: V(c,l) + $0.5N_2(g)$ = VN(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.444	55.753	55.753	0	125.000	117.262	-85.954
300	7.453	55.799	55.753	.014	124.996	117.214	-85.389
400	7.921	58.009	56.051	.783	124.804	114.649	-62.641
500	8.293	59.818	56.628	1.595	124.629	112.132	-49.012
600	8.556	61.355	57.292	2.438	124.465	109.648	-39.939
700	8.738	62.689	57.970	3.303	124.302	107.190	-33.466
800	8.865	63.864	58.634	4.184	124.135	104.757	-28.618
900	8.956	64.914	59.275	5.075	123.953	102.346	-24.853
1000	9.022	65.861	59.887	5.974	123.754	99.955	-21.845
1100	9.072	66.723	60.469	6.879	123.537	97.586	-19.388
1200	9.110	67.515	61.025	7.788	123.297	95.237	-17.345
1300	9.141	68.245	61.552	8.701	123.034	92.911	-15.619
1400	9.166	68.923	62.054	9.616	122.743	90.604	-14.144
1500	9.187	69.556	62.533	10.534	122.426	88.320	-12.868
1600	9.208	70.150	62.991	11.454	122.083	86.055	-11.754
1700	9.229	70.709	63.430	12.375	121.712	83.813	-10.775
1800	9.251	71.237	63.849	13.299	121.314	81.597	-9.907
1900	9.275	71.738	64.251	14.226	120.885	79.402	-9.133
2000	9.302	72.214	64.637	15.154	120.424	77.231	-8.439
2100	9.333	72.669	65.009	16.086	119.928	75.082	-7.814
2190	9.364	73.061	65.332	16.927	119.450	73.168	-7.302
2190	9.364	73.061	65.332	16.927	113.989	73.168	-7.302
2200	9.367	73.104	65.367	17.021	113.929	72.983	-7.250
2300	9.405	73.521	65.712	17.960	113.330	71.137	-6.759
2400	9.448	73.922	66.046	18.902	112.733	69.315	-6.312
2500	9.495	74.309	66.369	19.849	112.138	67.517	-5.902

*Data except enthalpy of formation at 298 K estimated.

Phase change: 2190 K, melting point of V; ΔH° = 5.461 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $Cp° = 8.618 + 0.406 \times 10^{-3}T - 1.151 \times 10^{5}T^{-2}$

$H° - H°_{298} = 8.618 \times 10^{-3}T + 0.203 \times 10^{-6}T^{2} + 1.151 \times 10^{2}T^{-1} - 2.974$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 124.581 + 0.249 \times 10^{-3}T - 1.204 \times 10^{-6}T^{2} + 134.750T^{-1}$

$\Delta Gf° = 124.581 - 0.249 \times 10^{-3}T\ln T + 1.204 \times 10^{-6}T^{2} + 67.375T^{-1} - 24.248 \times 10^{-3}T$

2000-2190 K: $\Delta Hf° = 125.918 - 0.816 \times 10^{-3}T - 0.937 \times 10^{-6}T^{2} - 415.200T^{-1}$

$\Delta Gf° = 125.918 + 0.816 \times 10^{-3}T\ln T + 0.937 \times 10^{-6}T^{2} - 207.600T^{-1} - 32.402 \times 10^{-3}T$

2190-2500 K: $\Delta Hf° = 128.122 - 6.748 \times 10^{-3}T + 0.175 \times 10^{-6}T^{2} - 430.900T^{-1}$

$\Delta Gf° = 128.122 + 6.748 \times 10^{-3}T\ln T - 0.175 \times 10^{-6}T^{2} - 215.450T^{-1} - 76.599 \times 10^{-3}T$

Source: Data from Chase (83) who estimated all except enthalpy of formation at 298 K.

$VOSO_4(c)$
Vanadyl Sulfate
[Reaction: $V(c) + 0.5S_2(g) + 2.5O_2(g) = VOSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15*	29.001	26.000	26.000	0	-328.255	-289.293	212.054
300	29.066	26.180	26.000	.054	-328.251	-289.050	210.570
400	32.344	35.001	27.181	3.128	-327.965	-276.021	150.809
500	35.174	42.531	29.515	6.508	-327.461	-263.087	114.994
600	37.555	49.161	32.248	10.148	-326.783	-250.273	91.161
700	39.487	55.101	35.095	14.004	-325.966	-237.585	74.176
800	40.970	60.475	37.938	18.030	-325.048	-225.023	61.473
900	42.005	65.365	40.717	22.183	-324.063	-212.577	51.620
1000	42.591	69.825	43.409	26.416	-323.052	-200.246	43.763
1100	42.728	73.894	45.998	30.686	-322.055	-188.011	37.354

*Data except enthalpy of formation and entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 28.833 + 15.628x10^{-3}T - 3.993x10^{5}T^{-2}$

$H°-H°_{298} = 28.833x10^{-3}T + 7.814x10^{-6}T^{2} + 3.993x10^{2}T^{-1} - 10.630$

Reaction equations (kcal/mol):

298.15-1100 K: $ΔHr° = -330.063 + 1.475x10^{-3}T + 5.285x10^{-6}T^{2} + 267.850T^{-1}$

$ΔGr° = -330.063 - 1.475x10^{-3}TlnT - 5.285x10^{-6}T^{2} + 133.925T^{-1} + 145.221x10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation and entropy at 298 K.

$VOSO_4 \cdot H_2O(c)$
Vanadyl Sulfate Monohydrate
[Reaction: $V(c) + 0.5S_2(g) + 3O_2(g) + H_2(g) = VOSO_4 \cdot H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	38.000	35.500	35.500	0	-402.905	-350.165	256.675
300	38.167	35.736	35.503	.070	-402.905	-349.838	254.853
350	42.667	41.957	35.983	2.091	-402.788	-341.000	212.928
400	47.167	47.948	37.106	4.337	-402.474	-332.192	181.499
450	51.667	53.763	38.634	6.808	-401.961	-323.435	157.079
500	56.167	59.440	40.432	9.504	-401.249	-314.746	137.573
550	60.667	65.004	42.413	12.425	-400.335	-306.137	121.646

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 10.880 + 90.528 \times 10^{-3}T + 0.115 \times 10^{5}T^{-2}$

$H° - H°_{298} = 10.880 \times 10^{-3}T + 45.264 \times 10^{-6}T^{2} - 0.115 \times 10^{2}T^{-1} - 7.229$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -398.229 - 26.549 \times 10^{-3}T + 42.064 \times 10^{-6}T^{2} - 149.050T^{-1}$

$\Delta Gr° = -398.229 + 26.549 \times 10^{-3}T\ln T - 42.064 \times 10^{-6}T^{2} - 74.525T^{-1} + 23.323 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$VOSO_4 \cdot 3H_2O(c)$
Vanadyl Sulfate Trihydrate
[Reaction: $V(c) + 0.5S_2(g) + 4O_2(g) + 3H_2(g) = VOSO_4 \cdot 3H_2O(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	57.000	54.500	54.500	0	-549.235	-468.941	343.738
300	57.244	54.853	54.500	.106	-549.238	-468.441	341.255
350	63.844	64.173	55.222	3.133	-549.160	-454.978	284.097
400	70.444	73.129	56.904	6.490	-548.788	-441.545	241.246
450	77.044	81.807	59.191	10.177	-548.121	-428.176	207.948
500	83.644	90.266	61.876	14.195	-547.154	-414.897	181.349
550	90.244	98.548	64.835	18.542	-545.888	-401.730	159.631

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 17.180 + 132.868 \times 10^{-3}T + 0.183 \times 10^{5}T^{-2}$
$H° - H°_{298} = 17.180 \times 10^{-3}T + 66.434 \times 10^{-6}T^{2} - 0.183 \times 10^{2}T^{-1} - 10.966$

Reaction equations (kcal/mol):

298.15-550 K: $ΔHr° = -542.131 - 40.391 \times 10^{-3}T + 61.893 \times 10^{-6}T^{2} - 168.050T^{-1}$
$ΔGr° = -542.131 + 40.391 \times 10^{-3}T\ln T - 61.893 \times 10^{-6}T^{2} - 84.025T^{-1} + 34.751 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$VOSO_4 \cdot 5H_2O(\alpha)$
α-Vanadyl Sulfate Pentahydrate
[Reaction: $V(c) + 0.5S_2(g) + 5O_2(g) + 5H_2(g) = VOSO_4 \cdot 5H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	76.000	73.500	73.500	0	-692.045	-584.196	428.222
300	76.333	73.971	73.501	.141	-692.052	-583.526	425.093
350	85.333	86.414	74.463	4.183	-692.004	-565.436	353.070
400	94.333	98.396	76.711	8.674	-691.551	-547.381	299.071
450	103.333	110.026	79.768	13.616	-690.690	-529.407	257.112
500	112.333	121.379	83.363	19.008	-689.417	-511.550	223.596
550	121.333	132.508	87.328	24.849	-687.731	-493.843	196.232

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 22.740 + 179.260 \times 10^{-3}T - 0.166 \times 10^{5}T^{-2}$
$H° - H°_{298} = 22.740 \times 10^{-3}T + 89.630 \times 10^{-6}T^{2} + 0.166 \times 10^{2}T^{-1} - 14.803$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -682.612 - 54.972 \times 10^{-3}T + 83.748 \times 10^{-6}T^{2} - 145.350T^{-1}$
$\Delta Gr° = -682.612 + 54.972 \times 10^{-3}T\ln T - 83.748 \times 10^{-6}T^{2} - 72.675T^{-1} + 42.666 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$VOSO_4 \cdot 5H_2O(\beta)$
β-Vanadyl Sulfate Pentahydrate
[Reaction: $V(c) + 0.5S_2(g) + 5O_2(g) + 5H_2(g) = VOSO_4 \cdot 5H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15*	76.000	73.500	73.500	0	-691.555	-583.706	427.862
300	76.333	73.971	73.501	.141	-691.562	-583.036	424.736
350	85.333	86.414	74.463	4.183	-691.514	-564.946	352.764
400	94.333	98.396	76.711	8.674	-691.061	-546.891	298.804
450	103.333	110.026	79.768	13.616	-690.200	-528.917	256.874
500	112.333	121.379	83.363	19.008	-688.927	-511.060	223.381
550	121.333	132.508	87.328	24.849	-687.241	-493.353	196.038

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 22.740 + 179.260 \times 10^{-3}T - 0.166 \times 10^{5}T^{-2}$

$H° - H°_{298} = 22.740 \times 10^{-3}T + 89.630 \times 10^{-6}T^{2} + 0.166 \times 10^{2}T^{-1} - 14.803$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -682.122 - 54.972 \times 10^{-3}T + 83.748 \times 10^{-6}T^{2} - 145.350T^{-1}$

$\Delta Gr° = -682.122 + 54.972 \times 10^{-3}T\ln T - 83.748 \times 10^{-6}T^{2} - 72.675T^{-1} + 42.666 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$VOSO_4 \cdot 6H_2O(c)$
Vanadyl Sulfate Hexahydrate
[Reaction: $V(c) + 0.5S_2(g) + 5.5O_2(g) + 6H_2(g) = VOSO_4 \cdot 6H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15*	85.000	83.000	83.000	0	-762.275	-640.648	469.602
300	85.388	83.527	83.000	.158	-762.284	-639.893	466.156
350	95.888	97.478	84.078	4.690	-762.269	-619.488	386.821
400	106.388	110.968	86.603	9.746	-761.778	-599.120	327.340
450	116.888	124.105	90.043	15.328	-760.807	-578.841	281.120
500	127.388	136.964	94.094	21.435	-759.352	-558.695	244.202
550	137.889	149.597	98.566	28.067	-757.413	-538.719	214.064

*Data except enthalpy or rormation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 22.683 + 209.504 \times 10^{-3}T - 0.131 \times 10^{5}T^{-2}$

$H° - H°_{298} = 22.683 \times 10^{-3}T + 104.752 \times 10^{-6}T^{2} + 0.131 \times 10^{2}T^{-1} - 16.119$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta H°r = -751.075 - 65.101 \times 10^{-3}T + 98.199 \times 10^{-6}T^{2} - 154.950T^{-1}$

$\Delta Gf° = -751.075 + 65.101 \times 10^{-3}T\ln T - 98.199 \times 10^{-6}T^{2} - 77.475T^{-1} + 29.606 \times 10^{-3}T$

Source: Data from DeKock (112) who estimated all except enthalpy of formation at 298 K.

$VSi_2(c,l)$
Vanadium Disilicide
[Formation: $V(c,l) + 2Si(c,l) = VSi_2(c,l)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	15.480	14.100	14.100	0	-28.900	-28.359	20.787
300	15.525	14.196	14.100	.029	-28.900	-28.355	20.656
400	17.100	18.910	14.733	1.671	-28.885	-28.180	15.397
500	17.853	22.815	15.971	3.422	-28.862	-28.004	12.240
600	18.303	26.113	17.393	5.232	-28.846	-27.836	10.139
700	18.629	28.960	18.847	7.079	-28.845	-27.670	8.639
800	18.906	31.465	20.270	8.956	-28.855	-27.497	7.512
900	19.168	33.707	21.640	10.860	-28.884	-27.324	6.635
1000	19.436	35.741	22.951	12.790	-28.921	-27.134	5.930
1100	19.720	37.606	24.199	14.748	-28.965	-26.967	5.358
1200	20.026	39.335	25.389	16.735	-29.015	-26.784	4.878
1300	20.358	40.951	26.525	18.754	-29.067	-26.597	4.471
1400	20.718	42.473	27.611	20.807	-29.123	-26.397	4.121
1500	21.110	43.915	28.650	22.898	-29.178	-26.221	3.820
1600	21.533	45.291	29.647	25.030	-29.227	-26.029	3.555
1687	21.931	46.441	30.484	26.921	-29.265	-25.812	3.344
1687	21.931	46.441	30.484	26.921	-53.429	-25.812	3.344
1700	21.990	46.610	30.606	27.206	-53.416	-25.590	3.290
1800	22.480	47.881	31.532	29.429	-53.311	-23.951	2.908
1900	23.003	49.110	32.424	31.703	-53.186	-22.322	2.568
1950	23.278	49.711	32.860	32.860	-53.115	-21.522	2.412
1950	46.000	68.532	32.860	69.560	-16.415	-21.522	2.412
2000	46.000	69.696	33.766	71.860	-15.210	-21.668	2.368

Phase changes: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.
1950 K, melting point of VSi_2; ΔH° = 36.700 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1950 K: $Cp° = 17.053 + 2.856\times10^{-3}T - 2.155\times10^{5}T^{-2}$
$H°-H°_{298} = 17.053\times10^{-3}T + 1.428\times10^{-6}T^{2} + 2.155\times10^{2}T^{-1} - 5.934$

1950-2100 K: $Cp° = 46.000$
$H°-H°_{298} = 46.000\times10^{-3}T - 20.140$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -29.155 + 0.584\times10^{-3}T - 0.386\times10^{-6}T^{2} + 34.200T^{-1}$
$\Delta Gf° = -29.155 - 0.584\times10^{-3}T\ln T + 0.386\times10^{-6}T^{2} + 17.100T^{-1} + 5.689\times10^{-3}T$

1687-1950 K: $\Delta Hf° = -54.013 - 0.258\times10^{-3}T + 0.316\times10^{-6}T^{2} + 231.200T^{-1}$
$\Delta Gf° = -54.013 + 0.258\times10^{-3}T\ln T - 0.316\times10^{-6}T^{2} + 115.600T^{-1} + 15.317\times10^{-3}T$

1950-2000 K: $\Delta Hf° = -68.219 + 28.689\times10^{-3}T - 1.112\times10^{-6}T^{2} + 15.700T^{-1}$
$\Delta Gf° = -68.219 - 28.689\times10^{-3}T\ln T + 1.112\times10^{-6}T^{2} + 7.850T^{-1} + 239.136\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Freund (161). Low-temperature heat capacities from Kalishevich (229). High-temperature data based on Kalishevich (230) and Bondarenko (50).

$V_3Si(c)$
Trivanadium Silicide
[Formation: $3V(c) + Si(c) = V_3Si(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	21.720	24.400	24.400	0	-39.600	-39.348	28.843
300	21.759	24.534	24.401	.040	-39.602	-39.346	28.663
400	23.091	31.005	25.272	2.293	-39.695	-39.249	21.445
500	23.666	36.228	26.960	4.634	-39.808	-39.125	17.102
560	23.855	38.921	28.100	6.060	-39.888	-39.038	15.235
560	24.419	39.010	28.100	6.110	-39.838	-39.038	15.235
600	24.613	40.701	28.883	7.091	-39.873	-38.979	14.198
700	25.100	44.532	30.852	9.576	-39.971	-38.826	12.122
800	25.586	47.915	32.776	12.111	-40.072	-38.653	10.559
900	26.073	50.957	34.630	14.694	-40.188	-38.466	9.341
1000	26.559	53.729	36.404	17.325	-40.318	-38.263	8.362
1100	27.046	56.284	38.098	20.005	-40.459	-38.059	7.561
1200	27.532	58.658	39.713	22.734	-40.621	-37.832	6.890
1300	28.018	60.881	41.256	25.512	-40.806	-37.592	6.320
1400	28.505	62.975	42.734	28.338	-41.022	-37.333	5.828
1500	28.991	64.958	44.149	31.213	-41.270	-37.070	5.401

Phase change: 560 K, α - β transition point of V_3Si; ΔH° = 0.050 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-560 K: $Cp° = 25.220 - 0.784x10^{-3}T - 2.905x10^{5}T^{-2}$
$H°- H°_{298} = 25.220x10^{-3}T - 0.392x10^{-6}T^{2} + 2.905x10^{2}T^{-1} - 8.459$
560-1500 K: $Cp° = 21.695 + 4.864x10^{-3}T$
$H°- H°_{298} = 21.695x10^{-3}T + 2.432x10^{-6}T^{2} - 6.802$

Formation equations (kcal/mol):

298.15-560 K: $ΔHf° = -41.294 + 4.208x10^{-3}T - 4.079x10^{-6}T^{2} + 239.100T^{-1}$
$ΔGf° = -41.294 - 4.208x10^{-3}TlnT + 4.079x10^{-6}T^{2} + 119.550T^{-1} + 27.941x10^{-3}T$
560-1500 K: $ΔHf° = -39.637 + 0.683x10^{-3}T - 1.255x10^{-6}T^{2} - 51.400T^{-1}$
$ΔGf° = -39.637 - 0.683x10^{-3}TlnT + 1.255x10^{-6}T^{2} - 25.700T^{-1} + 4.721x10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K form Freund (161) Low-temperature heat capacities from Surikov (487). High-temperature data fram Pankratz (386).

$WB(c)$
Tungsten Boride
[Formation: $W(c) + B(\beta) = WB(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	8.010	13.200	13.200	0	-15.900	-17.090	12.527
300	8.070	13.250	13.200	.020	-15.896	-17.090	12.450
400	10.370	15.940	13.565	.950	-15.874	-17.502	9.563
500	11.410	18.380	14.280	2.050	-15.787	-17.912	7.829
600	11.970	20.510	15.143	3.220	-15.710	-18.350	6.684
700	12.300	22.380	16.037	4.440	-15.634	-18.784	5.865
800	12.510	24.040	16.940	5.680	-15.572	-19.244	5.257
900	12.650	25.520	17.809	6.940	-15.522	-19.698	4.783
1000	12.740	26.860	18.650	8.210	-15.485	-20.165	4.407
1100	12.810	28.080	19.462	9.480	-15.472	-20.642	4.101
1200	12.850	29.190	20.215	10.770	-15.463	-21.103	3.843
1300	12.880	30.220	20.951	12.050	-15.486	-21.570	3.626
1400	12.900	31.180	21.651	13.340	-15.523	-22.033	3.439
1500	12.920	32.070	22.317	14.630	-15.582	-22.497	3.278

*Heat capacity and entropy at 298 K estimated. Data extrapolated above 1100 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 13.381 - 0.168\times10^{-3}T - 4.711\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 13.381\times10^{-3}T - 0.084\times10^{-6}T^{2} + 4.711\times10^{2}T^{-1} - 5.562$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf^\circ = -17.412 + 2.843\times10^{-3}T - 1.147\times10^{-6}T^{2} + 228.600T^{-1}$
$\Delta Gf^\circ = -17.412 - 2.843\times10^{-3}T\ln T + 1.147\times10^{-6}T^{2} + 114.300T^{-1} + 15.653\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Leonidov (299-300). Heat capacity and entropy at 298 K are those estimated by Mezaki (331). High-temperature data based on Mezaki (331). Data extrapolated above 1100 K.

$W_2B(c)$
Ditungsten Boride
[Formation: $2W(c) + B(\beta) = W_2B(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.360	28.200	28.200	0	-16.300	-19.636	14.394
300	15.410	28.290	28.200	.030	-16.297	-19.651	14.316
400	17.120	33.000	28.825	1.670	-16.156	-20.792	11.360
500	17.960	36.920	30.060	3.430	-16.015	-21.965	9.601
600	18.480	40.240	31.490	5.250	-15.906	-23.178	8.442
700	18.840	43.120	32.949	7.120	-15.806	-24.388	7.614
800	19.110	45.650	34.388	9.010	-15.726	-25.630	7.002
900	19.330	47.910	35.754	10.940	-15.647	-26.852	6.520
1000	19.530	49.960	37.080	12.880	-15.585	-28.105	6.142
1100	19.700	51.830	38.339	14.840	-15.535	-29.351	5.831
1200	19.860	53.550	39.533	16.820	-15.498	-30.618	5.576
1300	20.010	55.150	40.681	18.810	-15.480	-31.873	5.358
1400	20.150	56.640	41.769	20.820	-15.476	-33.116	5.170
1500	20.290	58.030	42.803	22.840	-15.491	-34.376	5.009

*Heat capacity and entropy at 298 K estimated. Data extrapolated above 1100 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 18.682 + 1.170\text{x}10^{-3}T - 3.253\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 18.682\text{x}10^{-3}T + 0.585\text{x}10^{-6}T^{2} + 3.253\text{x}10^{2}T^{-1} - 6.713$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = -17.126 + 2.329\text{x}10^{-3}T - 0.849\text{x}10^{-6}T^{2} + 61.800T^{-1}$

$\Delta Gf° = -17.126 - 2.329\text{x}10^{-3}T\ln T + 0.849\text{x}10^{-6}T^{2} + 30.900T^{-1} + 4.250\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Leonidov (298,300). Heat capacity and entropy at 298 K are those estimated by Mezaki (331). High-temperature data based on Mezaki (331). Data extrapolated above 1100 K.

$W_2B_5(c)$
Ditungsten Pentaboride
[Formation: $2W(c) + 5B(\beta) = W_2B_5(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	21.040	21.000	21.000	0	-47.700	-47.208	34.604
300	21.270	21.130	21.000	.040	-47.707	-47.197	34.383
400	29.600	28.560	21.960	2.640	-47.874	-47.006	25.683
500	33.570	35.640	24.000	5.820	-47.941	-46.771	20.443
600	35.830	41.970	26.470	9.300	-48.072	-46.542	16.953
700	37.290	47.610	29.096	12.960	-48.254	-46.259	14.443
800	38.310	52.660	31.735	16.740	-48.468	-45.964	12.557
900	39.080	57.220	34.320	20.610	-48.725	-45.629	11.080
1000	39.700	61.370	36.820	24.550	-49.015	-45.265	9.893
1100	40.220	65.180	39.225	28.550	-49.341	-44.886	8.918
1200	40.660	68.700	41.542	32.590	-49.720	-44.476	8.100
1300	41.060	71.970	43.755	36.680	-50.138	-43.989	7.395
1400	41.420	75.030	45.880	40.810	-50.606	-43.480	6.787
1500	41.760	77.900	47.927	44.960	-51.143	-42.953	6.258

*Heat capacity and entropy at 298 K estimated. Data extrapolated above 1100 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 39.098 + 2.266\times10^{-3}T - 16.655\times10^{5}T^{-2}$

$H° - H°_{298} = 39.098\times10^{-3}T + 1.133\times10^{-6}T^{2} + 16.655\times10^{2}T^{-1} - 17.344$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = -50.307 + 3.853\times10^{-3}T - 3.069\times10^{-6}T^{2} + 516.000T^{-1}$

$\Delta Gf° = -50.307 - 3.853\times10^{-3}T\ln T + 3.069\times10^{-6}T^{2} + 258.000T^{-1} + 28.528\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Leonidov (300). Heat capacity and entropy at 298 K are those estimated by Mezaki (331). High-temperature data based on Mezaki (331). Data extrapolated above 1100 K.

$WC(c)$
Tungsten Carbide
[Formation: $W(c) + C(c) = WC(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	8.460	7.672	7.672	0	-9.600	-9.153	6.709
300	8.497	7.724	7.672	.016	-9.599	-9.149	6.665
400	9.847	10.380	8.025	.942	-9.508	-9.011	4.923
500	10.526	12.657	8.729	1.964	-9.409	-8.899	3.890
600	10.945	14.616	9.551	3.039	-9.329	-8.808	3.208
700	11.242	16.326	10.399	4.149	-9.269	-8.723	2.723
800	11.477	17.843	11.237	5.285	-9.224	-8.651	2.363
900	11.678	19.207	12.048	6.443	-9.194	-8.578	2.083
1000	11.860	20.447	12.827	7.620	-9.169	-8.511	1.860
1100	12.030	21.585	13.571	8.815	-9.151	-8.426	1.674
1200	12.195	22.639	14.284	10.026	-9.140	-8.379	1.526
1300	12.357	23.622	14.966	11.253	-9.132	-8.312	1.397
1400	12.518	24.543	15.617	12.497	-9.126	-8.238	1.286
1500	12.680	25.412	16.241	13.757	-9.120	-8.180	1.192
1600	12.843	26.236	16.840	15.033	-9.113	-8.115	1.108
1700	13.009	27.020	17.416	16.326	-9.104	-8.047	1.034
1800	13.177	27.768	17.971	17.635	-9.093	-7.995	.971
1900	13.349	28.485	18.506	18.961	-9.077	-7.931	.912
2000	13.525	29.174	19.021	20.305	-9.058	-7.876	.861
2100	13.704	29.838	19.521	21.666	-9.034	-7.816	.813
2200	13.888	30.480	20.005	23.046	-9.002	-7.770	.772
2300	14.075	31.101	20.473	24.444	-8.964	-7.720	.734
2400	14.267	31.705	20.930	25.861	-8.920	-7.653	.697
2500	14.462	32.291	21.372	27.298	-8.867	-7.582	.663
2600	14.663	32.862	21.803	28.754	-8.808	-7.542	.634
2700	14.867	33.419	22.223	30.230	-8.739	-7.508	.608

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2700 K: $Cp° = 10.653 + 1.472\times10^{-3}T - 2.339\times10^{5}T^{-2}$

$H° - H°_{298} = 10.653\times10^{-3}T + 0.736\times10^{-6}T^{2} + 2.339\times10^{2}T^{-1} - 4.026$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -10.094 + 1.320\times10^{-3}T - 0.401\times10^{-6}T^{2} + 40.600T^{-1}$

$\Delta Gf° = -10.094 - 1.320\times10^{-3}T\ln T + 0.401\times10^{-6}T^{2} + 20.300T^{-1} + 10.330\times10^{-3}T$

2000-2700 K: $\Delta Hf° = -8.102 - 0.803\times10^{-3}T + 0.231\times10^{-6}T^{2} - 507.100T^{-1}$

$\Delta Gf° = -8.102 + 0.803\times10^{-3}T\ln T - 0.231\times10^{-6}T^{2} - 253.550T^{-1} - 5.470\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mah (317). Low-temperature heat capacities and entropy at 298 K from Andon (11). High-temperature data based on Andon (11), Chang (73), and Levinson (301).

$W_2C(c)$
Ditungsten Carbide
[Formation: $2W(c) + C(c) = W_2C(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	18.320	13.400	13.400	0	-6.300	-5.235	3.837
300	18.373	13.514	13.401	.034	-6.292	-5.227	3.808
400	20.325	19.101	14.149	1.981	-5.771	-4.946	2.702
500	21.368	23.759	15.619	4.070	-5.211	-4.807	2.101
600	22.053	27.718	17.313	6.243	-4.651	-4.785	1.743
700	22.570	31.158	19.051	8.475	-4.095	-4.845	1.513
800	22.996	34.201	20.759	10.754	-3.539	-4.997	1.365
900	23.370	36.931	22.405	13.073	-2.989	-5.203	1.263
1000	23.712	39.411	23.984	15.427	-2.432	-5.478	1.197
1100	24.032	41.687	25.492	17.814	-1.875	-5.783	1.149
1200	24.338	43.791	26.930	20.233	-1.318	-6.188	1.127
1300	24.634	45.751	28.303	22.682	-.757	-6.604	1.110
1400	24.922	47.587	29.616	25.160	-.196	-7.056	1.101
1500	25.205	49.316	30.872	27.666	.370	-7.576	1.104
1600	25.484	50.952	32.076	30.201	.941	-8.118	1.109
1700	25.760	52.505	33.233	32.763	1.517	-8.688	1.117
1800	26.033	53.985	34.345	35.352	2.097	-9.328	1.133
1900	26.304	55.400	35.416	37.969	2.686	-9.972	1.147
2000	26.573	56.756	36.450	40.613	3.278	-10.664	1.165

*Heat capacity at 298 K and data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.460 + 2.600\times10^{-3}T - 3.480\times10^{5}T^{-2}$
$H°-H°_{298} = 21.460\times10^{-3}T + 1.300\times10^{-6}T^{2} + 3.480\times10^{2}T^{-1} - 7.681$

Formation equations (kcal/mol):

298.15-2000 K: $ΔHf° = -8.612 + 6.312\times10^{-3}T - 0.208\times10^{-6}T^{2} + 133.700T^{-1}$
$ΔGf° = -8.612 - 6.312\times10^{-3}T\ln T + 0.208\times10^{-6}T^{2} + 66.850T^{-1} + 46.475\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mah (317). Entropy at 298 K based on Gupta (192). Heat capacity at 298 K and high-temperature data are those estimated by Schick (437).

$W(CO)_6(g)$
Tungsten Hexacarbonyl (ideal gas)
[Formation: $W(c) + 6C(c) + 3O_2(g) = W(CO)_6(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	49.892	119.814	119.814	0	-211.200	-198.310	145.363
300	50.006	120.123	119.816	.092	-211.182	-198.230	144.408
350	52.678	128.042	120.436	2.662	-210.637	-196.113	122.457
400	54.736	135.215	121.840	5.350	-210.109	-194.072	106.035
450	56.411	141.761	123.694	8.130	-209.621	-192.099	93.295
500	57.841	147.780	125.806	10.987	-209.173	-190.175	83.125
550	59.100	153.353	128.060	13.911	-208.775	-188.296	74.821
600	60.231	158.544	130.386	16.895	-208.410	-186.449	67.913

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 51.622 + 17.312\times10^{-3}T - 6.126\times10^{5}T^{-2}$

$H°- H°_{298} = 51.622\times10^{-3}T + 8.656\times10^{-6}T^{2} + 6.126\times10^{2}T^{-1} - 18.215$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = -210.353 + 3.009\times10^{-3}T + 2.180\times10^{-6}T^{2} - 577.800T^{-1}$

$\Delta Gf° = -210.353 - 3.009\times10^{-3}T\ln T - 2.180\times10^{-6}T^{2} - 288.900T^{-1} + 61.436\times10^{-3}T$

Source: Data from Pilcher (401).

WOF_4(c,l,g)
Tungsten Oxide Tetrafluoride
[Formation: $W(c) + 0.5O_2(g) + 2F_2(g) = WOF_4(c,l,g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	31.926	42.000	42.000	0	-336.260	-310.265	227.427
300	32.000	42.198	42.001	.059	-336.247	-310.103	225.907
379	35.600	50.071	42.847	2.738	-335.521	-303.286	174.887
379	43.500	53.237	42.847	3.938	-334.321	-303.286	174.887
400	43.500	55.583	43.456	4.851	-333.939	-301.578	164.772
460	43.500	61.663	45.443	7.461	-332.867	-296.801	141.011
460	26.807	90.820	45.443	20.873	-319.455	-296.801	141.011
500	27.504	93.084	49.166	21.959	-319.410	-294.834	128.870
600	28.622	98.205	56.923	24.769	-319.255	-289.937	105.608
700	29.369	102.676	63.146	27.671	-319.065	-285.061	88.999
800	29.887	106.634	68.339	30.636	-318.855	-280.223	76.552
900	30.259	110.177	72.795	33.644	-318.637	-275.400	66.875
1000	30.533	113.380	76.696	36.684	-318.415	-270.610	59.141
1100	30.742	116.300	80.165	39.748	-318.196	-265.830	52.815
1200	30.903	118.982	83.290	42.831	-317.981	-261.086	47.550
1300	31.030	121.461	86.132	45.928	-317.771	-256.346	43.095
1400	31.132	123.764	88.738	49.036	-317.573	-251.622	39.279
1500	31.215	125.915	91.146	52.154	-317.383	-246.922	35.976
1600	31.284	127.932	93.383	55.279	-317.203	-242.228	33.086
1700	31.341	129.830	95.471	58.410	-317.031	-237.537	30.537
1800	31.389	131.623	97.431	61.546	-316.874	-232.879	28.275
1900	31.430	133.321	99.275	64.687	-316.724	-228.212	26.250
2000	31.465	134.934	101.018	67.832	-316.590	-223.564	24.430

*Heat capacities 298 to 460 K estimated.

Phase changes: 379 K, melting point of WOF_4; ΔH° = 1.200 kcal/mol.
460 K, boiling point of WOF_4; ΔH° = 13.412 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-379 K: $Cp° = 17.624 + 47.970\times10^{-3}T$
$H°- H°_{298} = 17.624\times10^{-3}T + 23.985\times10^{-6}T^2 - 7.387$
379-460 K: $Cp° = 43.500$
$H°- H°_{298} = 43.500\times10^{-3}T - 12.549$
460-2000 K: $Cp° = 30.886 + 0.504\times10^{-3}T - 9.121\times10^5T^{-2}$
$H°- H°_{298} = 30.886\times10^{-3}T + 0.252\times10^{-6}T^2 + 9.121\times10^2T^{-1} + 4.629$

Formation equations (kcal/mol):

298.15-379 K: $\Delta Hf° = -334.855 - 8.822\times10^{-3}T + 23.014\times10^{-6}T^2 - 244.600T^{-1}$
$\Delta Gf° = -334.855 + 8.822\times10^{-3}T\ln T - 23.014\times10^{-6}T^2 - 122.300T^{-1} + 40.450\times10^{-3}T$
379-460 K: $\Delta Hf° = -340.017 + 17.054\times10^{-3}T - 0.971\times10^{-6}T^2 - 244.600T^{-1}$
$\Delta Gf° = -340.017 - 17.054\times10^{-3}T\ln T + 0.971\times10^{-6}T^2 - 122.300T^{-1} + 198.619\times10^{-3}T$
460-2000 K: $\Delta Hf° = -322.839 + 4.440\times10^{-3}T - 0.719\times10^{-6}T^2 + 667.500T^{-1}$
$\Delta Gf° = -322.839 - 4.440\times10^{-3}T\ln T + 0.719\times10^{-6}T^2 + 333.750T^{-1} + 81.896\times10^{-3}T$

Source: Data from Chase (81) who estimated heat capacities 298 to 460 K.

$WOF_4(g)$
Tungsten Oxide Tetrafluoride (ideal gas)
[Formation: $W(c) + 0.5O_2(g) + 2F_2(g) = WOF_4(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	22.909	79.969	79.969	0	-319.460	-304.785	223.411
300	22.974	80.111	79.971	.042	-319.464	-304.694	221.967
400	25.762	87.134	80.909	2.490	-319.500	-299.759	163.779
500	27.504	93.084	82.764	5.160	-319.409	-294.833	128.870
600	28.622	98.205	84.922	7.970	-319.254	-289.936	105.608
700	29.369	102.676	87.145	10.872	-319.063	-285.060	88.999
800	29.887	106.634	89.338	13.837	-318.853	-280.221	76.552
900	30.259	110.177	91.460	16.845	-318.635	-275.399	66.875
1000	30.533	113.380	93.495	19.885	-318.414	-270.609	59.141
1100	30.742	116.300	95.437	22.949	-318.194	-265.829	52.815
1200	30.903	118.982	97.289	26.032	-317.979	-261.085	47.549
1300	31.030	121.461	99.054	29.129	-317.770	-256.345	43.095
1400	31.132	123.764	100.738	32.237	-317.572	-251.621	39.279
1500	31.215	125.915	102.345	35.355	-317.381	-246.921	35.976
1600	31.284	127.932	103.882	38.480	-317.202	-242.227	33.086
1700	31.341	129.830	105.353	41.611	-317.030	-237.536	30.537
1800	31.389	131.623	106.764	44.747	-316.873	-232.878	28.275
1900	31.430	133.321	108.117	47.888	-316.723	-228.211	26.250
2000	31.465	134.934	109.418	51.033	-316.589	-223.563	24.429

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 29.414 + 1.458\text{x}10^{-3}T - 6.169\text{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 29.414\text{x}10^{-3}T + 0.729\text{x}10^{-6}T^2 + 6.169\text{x}10^{2}T^{-1} - 10.904$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -321.572 + 2.968\text{x}10^{-3}T - 0.242\text{x}10^{-6}T^2 + 372.300T^{-1}$

$\Delta Gf^\circ = -321.572 - 2.968\text{x}10^{-3}T\ln T + 0.242\text{x}10^{-6}T^2 + 186.150T^{-1} + 71.048\text{x}10^{-3}T$

Source: Data from Chase (81) who estimated some molecular constants.

WSi_2(c)
Tungsten Disilicide
[Formation: $W(c) + 2Si(c,l) = WSi_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.360	15.300	15.300	0	-22.200	-21.753	15.945
300	15.390	15.400	15.300	.030	-22.199	-21.749	15.844
400	16.360	19.970	15.920	1.620	-22.214	-21.602	11.803
500	16.950	23.690	17.110	3.290	-22.242	-21.442	9.372
600	17.390	26.820	18.470	5.010	-22.284	-21.282	7.752
700	17.760	29.530	19.873	6.760	-22.342	-21.117	6.593
800	18.090	31.920	21.220	8.560	-22.384	-20.928	5.717
900	18.410	34.070	22.537	10.380	-22.445	-20.744	5.037
1000	18.700	36.020	23.780	12.240	-22.486	-20.526	4.486
1100	18.990	37.820	24.984	14.120	-22.533	-20.344	4.042
1200	19.280	39.490	26.123	16.040	-22.563	-20.151	3.670
1300	19.560	41.040	27.209	17.980	-22.592	-19.940	3.352
1400	19.830	42.500	28.250	19.950	-22.615	-19.717	3.078
1500	20.100	43.880	29.253	21.940	-22.637	-19.547	2.848
1600	20.380	45.180	30.199	23.970	-22.638	-19.326	2.640
1687	20.615	46.272	31.007	25.752	-22.639	-19.109	2.476
1687	20.615	46.272	31.007	25.752	-46.803	-19.109	2.476
1700	20.650	46.430	31.124	26.020	-46.784	-18.887	2.428
1800	20.920	47.610	31.999	28.100	-46.635	-17.241	2.093
1900	21.180	48.750	32.855	30.200	-46.473	-15.617	1.796
2000	21.450	49.850	33.685	32.330	-46.290	-14.030	1.533

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2200 K: $Cp° = 16.212 + 2.638\times10^{-3}T - 1.456\times10^{5}T^{-2}$
$H°- H°_{298} = 16.212\times10^{-3}T + 1.319\times10^{-6}T^{2} + 1.456\times10^{2}T^{-1} - 5.439$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -21.693 - 0.961\times10^{-3}T + 0.246\times10^{-6}T^{2} - 72.400T^{-1}$
$\Delta Gf° = -21.693 + 0.961\times10^{-3}T\ln T - 0.246\times10^{-6}T^{2} - 36.200T^{-1} - 5.197\times10^{-3}T$
1687-2000 K: $\Delta Hf° = -46.551 - 1.803\times10^{-3}T + 0.948\times10^{-6}T^{2} + 124.600T^{-1}$
$\Delta Gf° = -46.551 + 1.803\times10^{-3}T\ln T - 0.948\times10^{-6}T^{2} + 62.300T^{-1} + 4.431\times10^{-3}T$

Source: Data from Chart (78).

W_5Si_3(c)
Pentatungsten Trisilicide
[Formation: $5W(c) + 3Si(c,l) = W_5Si_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	43.350	54.900	54.900	0	-32.200	-32.916	24.127
300	43.400	55.170	54.903	.080	-32.202	-32.916	23.979
400	45.370	67.940	56.615	4.530	-32.228	-33.148	18.111
500	46.780	78.230	59.950	9.140	-32.286	-33.376	14.588
600	47.980	86.860	63.727	13.880	-32.352	-33.606	12.241
700	49.070	94.340	67.583	18.730	-32.405	-33.798	10.552
800	50.110	100.960	71.348	23.690	-32.420	-34.004	9.289
900	51.120	106.920	74.976	28.750	-32.425	-34.180	8.300
1000	52.100	112.360	78.450	33.910	-32.374	-34.354	7.508
1100	53.080	117.370	81.761	39.170	-32.290	-34.534	6.861
1200	54.040	122.030	84.922	44.530	-32.172	-34.776	6.333
1300	55.000	126.390	87.944	49.980	-32.017	-34.968	5.879
1400	55.950	130.510	90.846	55.530	-31.833	-35.151	5.487
1500	56.910	134.400	93.620	61.170	-31.612	-35.452	5.165
1600	57.850	138.100	96.281	66.910	-31.351	-35.703	4.877
1687	58.676	141.189	98.524	71.976	-31.094	-35.856	4.645
1687	58.676	141.189	98.524	71.976	-67.340	-35.856	4.645
1700	58.800	141.640	98.852	72.740	-67.272	-35.601	4.577
1800	59.750	145.020	101.314	78.670	-66.727	-33.787	4.102
1900	60.690	148.280	103.706	84.690	-66.127	-31.965	3.677
2000	61.630	151.420	106.020	90.800	-65.482	-30.242	3.305

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2200 K: $Cp^{\circ} = 42.945 + 9.370\text{x}10^{-3}T - 2.122\text{x}10^{5}T^{-2}$

$H^{\circ} - H^{\circ}_{298} = 42.945\text{x}10^{-3}T + 4.685\text{x}10^{-6}T^{2} + 2.122\text{x}10^{2}T^{-1} - 13.932$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf^{\circ} = -30.782 - 3.167\text{x}10^{-3}T + 1.777\text{x}10^{-6}T^{2} - 188.300T^{-1}$

$\Delta Gf^{\circ} = -30.782 + 3.167\text{x}10^{-3}T\ln T - 1.777\text{x}10^{-6}T^{2} - 94.150T^{-1} - 23.611\text{x}10^{-3}T$

1687-2000 K: $\Delta Hf^{\circ} = -68.069 - 4.430\text{x}10^{-3}T + 2.830\text{x}10^{-6}T^{2} + 107.200T^{-1}$

$\Delta Gf^{\circ} = -68.069 + 4.430\text{x}10^{-3}T\ln T - 2.830\text{x}10^{-6}T^{2} + 53.600T^{-1} - 9.169\text{x}10^{-3}T$

Source: Data from Chart (78).

$YFeO_3(c)$
Yttrium Ferrite
[Formation: $Y(c) + Fe(c) + 1.5O_2(g) = YFeO_3(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	26.350	21.000	21.000	0	-331.500	-310.735	227.772
300	26.360	21.160	21.000	.050	-331.493	-310.603	226.271
400	27.250	28.860	22.060	2.720	-331.155	-303.703	165.933
500	28.480	35.070	24.050	5.510	-330.800	-296.873	129.761
600	29.830	40.380	26.347	8.420	-330.432	-290.124	105.676
700	31.250	45.080	28.680	11.480	-330.025	-283.430	88.490
800	32.700	49.350	31.000	14.680	-329.596	-276.801	75.618
900	34.170	53.280	33.258	18.020	-329.167	-270.230	65.620
1000	35.660	56.960	35.450	21.510	-328.798	-263.703	57.632

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 20.390 + 15.140\times10^{-3}T + 1.290\times10^{5}T^{-2}$

$H°-H°_{298} = 20.390\times10^{-3}T + 7.570\times10^{-6}T^{2} - 1.290\times10^{2}T^{-1} - 6.320$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -332.823 + 4.048\times10^{-3}T - 0.161\times10^{-6}T^{2} + 39.000T^{-1}$

$\Delta Gf° = -332.823 - 4.048\times10^{-3}T\ln T + 0.161\times10^{-6}T^{2} + 19.500T^{-1} + 96.883\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Tret'yakov (502) and Piekarczyk (399). Entropy at 298 K based on Vorob'ev (512) and Tret'yakov (502). High-temperature data from Kaul (237).

$Y_3Fe_5O_{12}$(c)
Yttrium Iron Oxide
[Formation: $3Y(c) + 5Fe(c) + 6O_2(g) = Y_3Fe_5O_{12}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	102.000	96.000	96.000	0	-1190.000	-1111.739	814.916
300	102.000	96.600	96.000	.200	-1189.969	-1111.231	809.521
400	115.000	128.100	100.350	11.100	-1188.382	-1085.298	592.972
500	119.800	154.300	108.500	22.900	-1186.349	-1059.698	463.188
560	130.800	168.400	114.114	30.400	-1184.930	-1044.539	407.644
600	121.600	177.000	118.000	35.400	-1184.083	-1034.526	376.821
700	121.800	195.800	127.943	47.500	-1182.699	-1009.826	315.278

Phase changes: 560 K, second-order transition point of $Y_3Fe_5O_{12}$; $\Delta H° = 0$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-560 K: $Cp° = 77.945 + 88.916\times10^{-3}T$
$H°- H°_{298} = 77.945\times10^{-3}T + 44.458\times10^{-6}T^2 - 27.191$
560-700 K: $Cp° = 91.857 + 57.140\times10^{-3}T$
$H°- H°_{298} = 91.857\times10^{-3}T + 28.570\times10^{-6}T^2 - 29.999$

Formation equations (kcal/mol):

298.15-560 K: $\Delta Hf° = -1199.260 + 18.516\times10^{-3}T + 8.370\times10^{-6}T^2 + 893.200T^{-1}$
$\Delta Gf° = -1199.260 - 18.516\times10^{-3}T\ln T - 8.370\times10^{-6}T^2 + 446.600T^{-1} + 396.518\times10^{-3}T$
560-700 K: $\Delta Hf° = -1202.068 + 32.428\times10^{-3}T - 7.518\times10^{-6}T^2 + 893.200T^{-1}$
$\Delta Gf° = -1202.068 - 32.428\times10^{-3}T\ln T + 7.518\times10^{-6}T^2 + 446.600T^{-1} + 480.669\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Piekarczyk (399). Entropy at 298 K and high-temperature data from Shchelkotunov (443).

YN(c)
Yttrium Nitride
[Formation: $Y(c,l) + 0.5N_2(g) = YN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	9.393	9.000	9.000	0	-71.500	-64.194	47.055
300	9.421	9.058	9.001	.017	-71.502	-64.149	46.732
400	10.426	11.924	9.384	1.016	-71.492	-61.698	33.710
500	10.975	14.314	10.138	2.088	-71.429	-59.254	25.900
600	11.344	16.349	11.007	3.205	-71.341	-56.825	20.698
700	11.628	18.120	11.900	4.354	-71.247	-54.416	16.989
800	11.867	19.689	12.778	5.529	-71.152	-52.016	14.210
900	12.079	21.099	13.626	6.726	-71.062	-49.635	12.053
1000	12.275	22.382	14.438	7.944	-70.976	-47.254	10.327
1100	12.460	23.561	15.215	9.181	-70.895	-44.893	8.919
1200	12.639	24.652	15.955	10.436	-70.821	-42.530	7.746
1300	12.812	25.671	16.665	11.708	-70.753	-40.175	6.754
1400	12.981	26.627	17.343	12.998	-70.689	-37.818	5.904
1500	13.147	27.528	17.992	14.304	-70.632	-35.481	5.169
1600	13.312	28.382	18.615	15.627	-70.580	-33.140	4.527
1700	13.474	29.193	19.212	16.967	-70.530	-30.793	3.959
1752	13.558	29.600	19.515	17.669	-70.511	-29.576	3.689
1752	13.558	29.600	19.515	17.669	-71.704	-29.576	3.689
1799	13.634	29.960	19.783	18.308	-71.657	-28.454	3.457
1799	13.634	29.960	19.783	18.308	-74.381	-28.454	3.457
1800	13.636	29.968	19.789	18.322	-74.382	-28.424	3.451
1900	13.797	30.710	20.345	19.694	-74.466	-25.864	2.975
2000	13.956	31.422	20.881	21.082	-74.537	-23.320	2.548

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1752 K, α - β transition point of Y; ΔH° = 1.193 kcal/mol.
1799 K, melting point of Y; ΔH° = 2.724 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.900 + 1.550\times10^{-3}T - 1.750\times10^{5}T^{-2}$
$H°-H°_{298} = 10.900\times10^{-3}T + 0.775\times10^{-6}T^{2} + 1.750\times10^{2}T^{-1} - 3.906$

Formation equations (kcal/mol):

298.15-1752 K: $\Delta Hf° = -72.660 + 1.923\times10^{-3}T - 0.424\times10^{-6}T^{2} + 186.250T^{-1}$
$\Delta Gf° = -72.660 - 1.923\times10^{-3}T\ln T + 0.424\times10^{-6}T^{2} + 93.125T^{-1} + 38.182\times10^{-3}T$
1752-1799 K: $\Delta Hf° = -71.998 - 0.719\times10^{-3}T + 0.481\times10^{-6}T^{2} + 178.950T^{-1}$
$\Delta Gf° = -71.998 + 0.719\times10^{-3}T\ln T - 0.481\times10^{-6}T^{2} + 89.475T^{-1} + 19.659\times10^{-3}T$
1799-2000 K: $\Delta Hf° = -71.232 - 2.659\times10^{-3}T + 0.481\times10^{-6}T^{2} + 178.950T^{-1}$
$\Delta Gf° = -71.232 + 2.659\times10^{-3}T\ln T - 0.481\times10^{-6}T^{2} + 89.475T^{-1} + 4.693\times10^{-3}T$

Source: Data from Barin (23) who estimated all except enthalpy of formation at 298 K.

YO(g)
Yttrium Monoxide (ideal gas)
[Formation: $Y(c,l) + 0.5O_2(g) = YO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHf°	ΔGf°	
298.15	7.540	55.875	55.875	0	-11.000	-17.187	12.599
300	7.540	55.922	55.875	.014	-11.005	-17.226	12.549
400	7.910	58.143	56.176	.787	-11.227	-19.267	10.527
500	8.190	59.941	56.755	1.593	-11.444	-21.249	9.288
600	8.390	61.453	57.415	2.423	-11.665	-23.187	8.446
700	8.520	62.757	58.087	3.269	-11.899	-25.093	7.834
800	8.620	63.902	58.744	4.126	-12.149	-26.959	7.365
900	8.690	64.922	59.375	4.992	-12.418	-28.800	6.993
1000	8.740	65.840	59.976	5.864	-12.704	-30.599	6.687
1100	8.790	66.675	60.548	6.740	-13.010	-32.381	6.433
1200	8.820	67.442	61.091	7.621	-13.334	-34.127	6.215
1300	8.850	68.149	61.607	8.504	-13.677	-35.845	6.026
1400	8.870	68.805	62.098	9.390	-14.038	-37.528	5.858
1500	8.890	69.418	62.566	10.278	-14.421	-39.203	5.712
1600	8.910	69.993	63.013	11.168	-14.821	-40.843	5.579
1700	8.920	70.533	63.439	12.060	-15.239	-42.449	5.457
1752	8.930	70.802	63.654	12.524	-15.468	-43.276	5.398
1752	8.930	70.802	63.654	12.524	-16.661	-43.276	5.398
1799	8.940	71.039	63.844	12.944	-16.843	-43.995	5.345
1799	8.940	71.039	63.844	12.944	-19.567	-43.995	5.345
1800	8.940	71.044	63.848	12.953	-19.573	-44.004	5.343
1900	8.950	71.527	64.239	13.847	-20.156	-45.340	5.215
2000	8.960	71.986	64.615	14.742	-20.741	-46.666	5.099

Phase changes: 1752 K, α - β transition point of Y; ΔH° = 1.193 kcal/mol.
1799 K, melting point of Y; ΔH° = 2.724 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.382 + 0.382\times10^{-3}T - 0.850\times10^{5}T^{-2}$
$H° - H°_{298} = 8.382\times10^{-3}T + 0.191\times10^{-6}T^{2} + 0.850\times10^{2}T^{-1} - 2.801$

Formation equations (kcal/mol):

298.15-1752 K: $\Delta Hf° = -10.864 - 0.951\times10^{-3}T - 0.965\times10^{-6}T^{2} + 69.700T^{-1}$
$\Delta Gf° = -10.864 + 0.951\times10^{-3}T\ln T + 0.965\times10^{-6}T^{2} + 34.850T^{-1} - 27.306\times10^{-3}T$
1752-1799 K: $\Delta Hf° = -10.202 - 3.593\times10^{-3}T - 0.060\times10^{-6}T^{2} + 62.400T^{-1}$
$\Delta Gf° = -10.202 + 3.593\times10^{-3}T\ln T + 0.060\times10^{-6}T^{2} + 31.200T^{-1} - 45.829\times10^{-3}T$
1799-2000 K: $\Delta Hf° = -9.436 - 5.533\times10^{-3}T - 0.060\times10^{-6}T^{2} + 62.400T^{-1}$
$\Delta Gf° = -9.436 + 5.533\times10^{-3}T\ln T + 0.060\times10^{-6}T^{2} + 31.200T^{-1} - 60.795\times10^{-3}T$

Source: Data from Pedley (396).

$YO_2(g)$
Yttrium Dioxide (ideal gas)
[Formation: $Y(c,l) + O_2(g) = YO_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.645	65.037	65.037	0	-104.478	-106.092	77.766
300	10.667	65.103	65.037	.020	-104.483	-106.101	77.294
400	11.665	68.318	65.468	1.140	-104.714	-106.605	58.246
500	12.309	70.996	66.314	2.341	-104.901	-107.053	46.792
600	12.726	73.279	67.289	3.594	-105.076	-107.465	39.144
700	13.005	75.263	68.290	4.881	-105.258	-107.853	33.673
800	13.199	77.013	69.273	6.192	-105.454	-108.208	29.561
900	13.338	78.576	70.222	7.519	-105.668	-108.545	26.358
1000	13.441	79.987	71.128	8.859	-105.900	-108.847	23.788
1100	13.518	81.272	71.993	10.207	-106.153	-109.136	21.683
1200	13.579	82.451	72.816	11.562	-106.427	-109.395	19.923
1300	13.626	83.540	73.600	12.922	-106.721	-109.629	18.430
1400	13.664	84.551	74.346	14.287	-107.036	-109.833	17.146
1500	13.695	85.495	75.058	15.655	-107.373	-110.031	16.031
1600	13.720	86.380	75.739	17.025	-107.732	-110.198	15.052
1700	13.742	87.212	76.390	18.398	-108.110	-110.334	14.184
1752	13.751	87.626	76.717	19.114	-108.318	-110.395	13.771
1752	13.751	87.626	76.717	19.114	-109.511	-110.395	13.771
1799	13.760	87.990	77.006	19.760	-109.676	-110.423	13.414
1799	13.760	87.990	77.006	19.760	-112.400	-110.423	13.414
1800	13.760	87.998	77.012	19.774	-112.405	-110.418	13.406
1900	13.775	88.743	77.611	21.150	-112.953	-110.289	12.686
2000	13.788	89.449	78.185	22.528	-113.504	-110.150	12.036

Phase changes: 1752 K, α - β transition point of Y; ΔH° = 1.193 kcal/mol.
1799 K, melting point of Y; ΔH° = 2.724 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.979 + 0.574\times10^{-3}T - 2.227\times10^{5}T^{-2}$
$H°- H°_{298} = 12.979\times10^{-3}T + 0.287\times10^{-6}T^{2} + 2.227\times10^{2}T^{-1} - 4.642$

Formation equations (kcal/mol):

298.15-1752 K: $\Delta Hf° = -105.007 + 0.031\times10^{-3}T - 1.121\times10^{-6}T^{2} + 184.800T^{-1}$
$\Delta Gf° = -105.007 - 0.031\times10^{-3}T\ln T + 1.121\times10^{-6}T^{2} + 92.400T^{-1} - 4.833\times10^{-3}T$
1752-1799 K: $\Delta Hf° = -104.345 - 2.611\times10^{-3}T - 0.216\times10^{-6}T^{2} + 177.500T^{-1}$
$\Delta Gf° = -104.345 + 2.611\times10^{-3}T\ln T + 0.216\times10^{-6}T^{2} + 88.750T^{-1} - 23.356\times10^{-3}T$
1799-2000 K: $\Delta Hf° = -103.579 - 4.551\times10^{-3}T - 0.216\times10^{-6}T^{2} + 177.500T^{-1}$
$\Delta Gf° = -103.579 + 4.551\times10^{-3}T\ln T + 0.216\times10^{-6}T^{2} + 88.750T^{-1} - 38.322\times10^{-3}T$

Source: Data from Gurvich (196).

$Y_2O(g)$
Diyttrium Oxide (ideal gas)
[Formation: $2Y(c,l) + 0.5O_2(g) = Y_2O(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.539	68.915	68.915	0	-.515	-7.424	5.442
300	11.555	68.987	68.917	.021	-.525	-7.467	5.440
400	12.267	72.416	69.379	1.215	-.967	-9.716	5.308
500	12.728	75.206	70.274	2.466	-1.396	-11.849	5.179
600	13.031	77.555	71.297	3.755	-1.831	-13.894	5.061
700	13.235	79.581	72.340	5.069	-2.288	-15.877	4.957
800	13.378	81.358	73.358	6.400	-2.773	-17.780	4.857
900	13.481	82.940	74.336	7.744	-3.291	-19.635	4.768
1000	13.557	84.364	75.268	9.096	-3.842	-21.411	4.679
1100	13.615	85.659	76.155	10.454	-4.427	-23.154	4.600
1200	13.660	86.846	76.998	11.818	-5.049	-24.828	4.522
1300	13.696	87.941	77.798	13.186	-5.706	-26.446	4.446
1400	13.724	88.957	78.559	14.557	-6.399	-28.001	4.371
1500	13.748	89.904	79.283	15.931	-7.130	-29.536	4.303
1600	13.767	90.792	79.975	17.307	-7.896	-31.004	4.235
1700	13.783	91.627	80.636	18.684	-8.698	-32.413	4.167
1752	13.790	92.043	80.970	19.401	-9.138	-33.128	4.132
1752	13.790	92.043	80.970	19.401	-11.524	-33.128	4.132
1799	13.796	92.408	81.264	20.049	-11.870	-33.718	4.096
1799	13.796	92.408	81.264	20.049	-17.318	-33.718	4.096
1800	13.796	92.416	81.270	20.063	-17.329	-33.718	4.094
1900	13.808	93.162	81.876	21.443	-18.456	-34.586	3.978
2000	13.818	93.870	82.458	22.825	-19.583	-35.438	3.872

Phase changes: 1752 K, α - β transition point of Y; ΔH° = 1.193 kcal/mol.
1799 K, melting point of Y; ΔH° = 2.724 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.200 + 0.434\times10^{-3}T - 1.592\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 13.200\times10^{-3}T + 0.217\times10^{-6}T^2 + 1.592\times10^{2}T^{-1} - 4.489$

Formation equations (kcal/mol):

298.15-1752 K: $\Delta Hf^\circ = -0.306 - 1.851\times10^{-3}T - 1.845\times10^{-6}T^2 + 151.200T^{-1}$
$\Delta Gf^\circ = -0.306 + 1.851\times10^{-3}T\ln T + 1.845\times10^{-6}T^2 + 75.600T^{-1} - 35.819\times10^{-3}T$
1752-1799 K: $\Delta Hf^\circ = 1.018 - 7.135\times10^{-3}T - 0.034\times10^{-6}T^2 + 136.600T^{-1}$
$\Delta Gf^\circ = 1.018 + 7.135\times10^{-3}T\ln T + 0.034\times10^{-6}T^2 + 68.300T^{-1} - 72.865\times10^{-3}T$
1799-2000 K: $\Delta Hf^\circ = 2.550 - 11.015\times10^{-3}T - 0.034\times10^{-6}T^2 + 136.600T^{-1}$
$\Delta Gf^\circ = 2.550 + 11.015\times10^{-3}T\ln T + 0.034\times10^{-6}T^2 + 68.300T^{-1} - 102.797\times10^{-3}T$

Source: Data from Gurvich (196).

$Y_2O_2(g)$
Diyttrium Dioxide (ideal gas)
[Formation: $2Y(c,l) + O_2(g) = Y_2O_2(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.107	71.671	71.671	0	-133.089	-133.514	97.867
300	14.138	71.758	71.671	.026	-133.100	-133.517	97.266
400	15.625	76.039	72.244	1.518	-133.600	-133.580	72.984
500	16.705	79.649	73.375	3.137	-134.026	-133.520	58.361
600	17.462	82.766	74.686	4.848	-134.416	-133.377	48.582
700	17.995	85.500	76.040	6.622	-134.802	-133.181	41.580
800	18.377	87.929	77.377	8.442	-135.198	-132.917	36.311
900	18.658	90.110	78.672	10.294	-135.614	-132.618	32.204
1000	18.868	92.087	79.916	12.171	-136.054	-132.251	28.903
1100	19.030	93.894	81.107	14.066	-136.522	-131.862	26.198
1200	19.156	95.555	82.242	15.976	-137.022	-131.414	23.934
1300	19.256	97.092	83.325	17.897	-137.553	-130.922	22.010
1400	19.337	98.523	84.362	19.826	-138.120	-130.378	20.353
1500	19.403	99.859	85.350	21.764	-138.722	-129.821	18.915
1600	19.458	101.113	86.296	23.707	-139.360	-129.206	17.649
1700	19.504	102.294	87.203	25.655	-140.032	-128.540	16.525
1752	19.524	102.882	87.660	26.669	-140.405	-128.178	15.989
1752	19.524	102.882	87.660	26.669	-142.791	-128.178	15.989
1799	19.543	103.399	88.064	27.587	-143.077	-127.796	15.525
1799	19.543	103.399	88.064	27.587	-148.525	-127.796	15.525
1800	19.543	103.410	88.073	27.607	-148.534	-127.776	15.514
1900	19.576	104.468	88.909	29.563	-149.532	-126.586	14.560
2000	19.604	105.472	89.711	31.522	-150.532	-125.384	13.701

Phase changes: 1752 K, α - β transition point of Y; ΔH° = 1.193 kcal/mol.
1799 K, melting point of Y; ΔH° = 2.724 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 17.521 + 1.426\times10^{-3}T - 3.413\times10^{5}T^{-2}$
$H°- H°_{298} = 17.521\times10^{-3}T + 0.713\times10^{-6}T^{2} + 3.413\times10^{2}T^{-1} - 6.432$

Formation equations (kcal/mol):

298.15-1752 K: $\Delta Hf° = -133.647 - 1.145\times10^{-3}T - 1.600\times10^{-6}T^{2} + 310.700T^{-1}$
$\Delta Gf° = -133.647 + 1.145\times10^{-3}T\ln T + 1.600\times10^{-6}T^{2} + 155.350T^{-1} - 8.301\times10^{-3}T$
1752-1799 K: $\Delta Hf° = -132.323 - 6.429\times10^{-3}T + 0.210\times10^{-6}T^{2} + 296.100T^{-1}$
$\Delta Gf° = -132.323 + 6.429\times10^{-3}T\ln T - 0.210\times10^{-6}T^{2} + 148.050T^{-1} - 45.347\times10^{-3}T$
1799-2000 K: $\Delta Hf° = -130.791 - 10.309\times10^{-3}T + 0.210\times10^{-6}T^{2} + 296.100T^{-1}$
$\Delta Gf° = -130.791 + 10.309\times10^{-3}T\ln T - 0.210\times10^{-6}T^{2} + 148.050T^{-1} - 75.279\times10^{-3}T$

Source: Data from Gurvich (196).

$Y_2WO_6(c)$
Yttrium Tungstate
[Formation: $2Y(c) + W(c) + 3O_2(g) = Y_2WO_6(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	41.290	36.730	36.730	0	-693.100	-651.560	477.600
300	41.460	36.990	36.730	.080	-693.094	-651.299	474.465
400	47.720	49.880	38.455	4.570	-692.607	-637.435	348.274
500	51.150	60.930	41.870	9.530	-691.760	-623.728	272.628
600	53.450	70.470	45.853	14.770	-690.749	-610.210	222.266
700	55.230	78.850	49.993	20.200	-689.661	-596.884	186.353
800	56.730	86.320	54.070	25.800	-688.505	-583.705	159.459
900	58.060	93.080	58.036	31.540	-687.302	-570.683	138.579
1000	59.290	99.260	61.850	37.410	-686.048	-557.778	121.901
1100	60.460	104.970	65.515	43.400	-684.752	-545.019	108.284
1200	61.580	110.280	69.030	49.500	-683.420	-532.383	96.959
1300	62.660	115.250	72.396	55.710	-682.043	-519.843	87.392
1400	63.730	119.930	75.623	62.030	-680.626	-507.391	79.206
1500	64.780	124.360	78.720	68.460	-679.162	-495.083	72.133

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 50.620 + 9.760\times10^{-3}T - 10.880\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 50.620\times10^{-3}T + 4.880\times10^{-6}T^{2} + 10.880\times10^{2}T^{-1} - 19.175$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf^\circ = -699.861 + 11.679\times10^{-3}T + 1.190\times10^{-6}T^{2} + 946.000T^{-1}$

$\Delta Gf^\circ = -699.861 - 11.679\times10^{-3}T\ln T - 1.190\times10^{-6}T^{2} + 473.000T^{-1} + 223.577\times10^{-3}T$

Source: Data based on Abashidze (1).

$Y_2W_3O_{12}$(c)
Yttrium Tritungstate
[Formation: $2Y(c) + 3W(c) + 6O_2(g) = Y_2W_3O_{12}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	71.760	83.690	83.690	0	-1100.800	-1024.778	751.173
300	72.140	84.130	83.697	.130	-1100.805	-1024.304	746.195
400	85.770	107.010	86.710	8.120	-1100.130	-998.870	545.750
500	92.750	126.970	92.830	17.070	-1098.698	-973.715	425.605
600	97.110	144.290	99.990	26.580	-1096.918	-948.885	345.627
700	100.230	159.510	107.424	36.460	-1094.966	-924.358	288.594
800	102.690	173.060	114.798	46.610	-1092.918	-900.134	245.902
900	104.770	185.270	121.959	56.980	-1090.809	-876.155	212.757
1000	106.610	196.410	128.860	67.550	-1088.626	-852.416	186.293
1100	108.300	206.650	135.468	78.300	-1086.393	-828.883	164.682
1200	109.880	216.140	141.798	89.210	-1084.119	-805.589	146.716
1300	111.380	225.000	147.869	100.270	-1081.798	-782.463	131.542
1400	112.840	233.300	153.671	111.480	-1079.441	-759.474	118.558
1500	114.250	241.140	159.247	122.840	-1077.029	-736.742	107.342

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 96.720 + 12.440x10^{-3}T - 25.480x10^{5}T^{-2}$

$H°- H°_{298} = 96.720x10^{-3}T + 6.220x10^{-6}T^{2} + 25.480x10^{2}T^{-1} - 37.936$

Formation equations (kcal/mol):

298.15-1500 K: $ΔHf° = -1115.591 + 24.459x10^{-3}T + 0.279x10^{-6}T^{2} + 2228.400T^{-1}$

$ΔGf° = -1115.591 - 24.459x10^{-3}TlnT - 0.279x10^{-6}T^{2} + 1114.200T^{-1} + 431.497x10^{-3}T$

Source: Data based on Abashidze (1).

Y_6WO_{12}(c)
Triyttrium Tungstate
[Formation: $6Y(c) + W(c) + 6O_2(g) = Y_6WO_{12}(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	86.338	92.580	92.580	0	-1600.800	-1519.414	1113.746
300	86.638	93.115	92.582	.160	-1600.801	-1518.907	1106.509
400	97.728	119.755	96.137	9.447	-1600.211	-1491.681	815.006
500	103.680	142.257	103.173	19.542	-1599.050	-1464.661	640.194
600	107.610	161.527	111.332	30.117	-1597.661	-1437.902	523.749
700	110.585	178.347	119.730	41.032	-1596.186	-1411.408	440.656
800	113.052	193.279	128.008	52.217	-1594.675	-1385.106	378.389
900	115.222	206.722	136.019	63.633	-1593.146	-1359.027	330.013
1000	117.209	218.966	143.710	75.256	-1591.600	-1333.066	291.338
1100	119.076	230.226	151.071	87.071	-1590.044	-1307.318	259.737
1200	120.861	240.664	158.107	99.068	-1588.483	-1281.686	233.424
1300	122.588	250.406	164.836	111.241	-1586.903	-1256.167	211.178
1400	124.274	259.553	171.279	123.584	-1585.319	-1230.734	192.124
1500	125.929	268.184	177.454	136.095	-1583.724	-1205.523	175.642

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^{\circ} = 103.923 + 15.254\times10^{-3}T - 19.675\times10^{5}T^{-2}$

$H^{\circ}- H^{\circ}_{298} = 103.923\times10^{-3}T + 7.627\times10^{-6}T^{2} + 19.675\times10^{2}T^{-1} - 38.262$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf^{\circ} = -1612.548 + 20.420\times10^{-3}T - 1.192\times10^{-6}T^{2} + 1719.100T^{-1}$

$\Delta Gf^{\circ} = -1612.548 - 20.420\times10^{-3}T\ln T + 1.192\times10^{-6}T^{2} + 859.550T^{-1} + 418.694\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Abashidze (1). High-temperature data based on Abashidze (2).

$Y_{10}W_2O_{21}$(c)
Pentayttrium Ditungstate
[Formation: 10Y(c) + 2W(c) + 10.5O_2(g) = $Y_{10}W_2O_{21}$(c)]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15	137.108	155.860	155.860	0	-2750.300	-2607.041	1910.988
300	138.017	156.711	155.864	.254	-2750.325	-2606.150	1898.554
400	169.945	201.447	161.745	15.881	-2749.744	-2558.113	1397.670
500	184.706	241.139	173.747	33.696	-2747.387	-2510.431	1097.295
600	192.710	275.589	187.917	52.603	-2744.374	-2463.304	897.246
700	197.524	305.685	202.638	72.133	-2741.175	-2416.736	754.529
800	200.637	332.278	217.213	92.052	-2737.989	-2370.595	647.608
900	202.761	356.040	231.342	112.228	-2734.912	-2324.899	564.555
1000	204.272	377.486	244.902	132.584	-2731.979	-2279.450	498.167
1100	205.382	397.009	257.855	153.069	-2729.229	-2234.377	443.924
1200	206.218	414.917	270.208	173.651	-2726.686	-2189.509	398.759
1300	206.862	431.450	281.984	194.306	-2724.337	-2144.814	360.571
1400	207.367	446.799	293.214	215.019	-2722.214	-2100.225	327.856
1500	207.767	461.120	303.936	235.776	-2720.314	-2055.969	299.551
1600	208.090	474.540	314.184	256.570	-2718.638	-2011.727	274.786

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp^\circ = 211.161 - 0.314\times10^{-3}T - 65.745\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 211.161\times10^{-3}T - 0.157\times10^{-6}T^{2} + 65.745\times10^{2}T^{-1} - 84.995$

Formation equations (kcal/mol):

298.15-1600 K: $\Delta Hf^\circ = -2789.317 + 66.436\times10^{-3}T - 15.231\times10^{-6}T^{2} + 6130.900T^{-1}$

$\Delta Gf^\circ = -2789.317 - 66.436\times10^{-3}T\ln T + 15.231\times10^{-6}T^{2} + 3065.450T^{-1} + 950.856\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Abashidze (1). High-temperature data based on Abashidze (2).

$Y_{14}W_4O_{33}(c)$
Heptayttrium Tetratungstate
[Formation: $14Y(c) + 4W(c) + 16.5O_2(g) = Y_{14}W_4O_{33}(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	224.510	232.640	232.640	0	-4133.000	-3907.652	2864.349
300	225.530	234.030	232.640	.420	-4133.006	-3906.243	2845.659
400	262.430	304.680	242.030	25.060	-4131.419	-3830.833	2093.043
500	280.750	365.410	260.790	52.310	-4127.853	-3756.040	1641.743
600	291.740	417.640	282.690	80.970	-4123.544	-3682.064	1341.174
700	299.290	463.210	305.296	110.540	-4118.989	-3608.875	1126.727
800	304.990	503.560	327.598	140.770	-4114.380	-3536.300	966.060
900	309.620	539.760	349.193	171.510	-4109.813	-3464.366	841.252
1000	313.590	572.590	369.920	202.670	-4105.309	-3392.824	741.492
1100	317.120	602.640	389.722	234.210	-4100.893	-3321.834	659.979
1200	320.360	630.380	408.638	266.090	-4096.586	-3251.220	592.120
1300	323.390	656.140	426.694	298.280	-4092.368	-3180.894	534.750
1400	326.260	680.210	443.953	330.760	-4088.284	-3110.798	485.611
1500	329.030	702.820	460.473	363.520	-4084.313	-3041.282	443.109

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 297.729 + 22.976\times10^{-3}T - 71.179\times10^{5}T^{-2}$

$H°- H°_{298} = 297.729\times10^{-3}T + 11.488\times10^{-6}T^{2} + 71.179\times10^{2}T^{-1} - 113.663$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = -4175.856 + 75.122\times10^{-3}T - 10.965\times10^{-6}T^{2} + 6390.300T^{-1}$

$\Delta Gf° = -4175.856 - 75.122\times10^{-3}T\ln T + 10.965\times10^{-6}T^{2} + 3195.150T^{-1} + 1288.36\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Abashidze (1). High-temperature data based on Abashidze (2).

YbN(c)
Ytterbium Nitride
[Formation: $Yb(c,l,g) + 0.5N_2(g) = YbN(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	14.000	16.000	16.000	0	-86.900	-80.584	59.069
300	14.010	16.087	16.000	.030	-86.889	-80.541	58.673
400	14.140	20.134	16.559	1.430	-86.484	-78.494	42.887
500	14.280	23.300	17.600	2.850	-86.109	-76.537	33.454
553	14.349	24.747	18.211	3.614	-85.948	-75.528	29.849
600	14.410	25.920	18.770	4.290	-85.775	-74.650	27.191
700	14.540	28.150	19.950	5.740	-85.407	-72.818	22.735
800	14.680	30.100	21.100	7.200	-85.049	-71.050	19.410
900	14.820	31.840	22.207	8.670	-84.703	-69.325	16.834
1000	14.950	33.410	23.250	10.160	-84.356	-67.642	14.783
1033	14.993	33.896	23.582	10.654	-84.245	-67.090	14.194
1033	14.993	33.896	23.582	10.654	-84.663	-67.090	14.194
1097	15.076	34.799	24.211	11.615	-84.508	-66.001	13.149
1097	15.076	34.799	24.211	11.615	-86.338	-66.001	13.149
1100	15.080	34.840	24.240	11.660	-86.330	-65.948	13.102
1200	15.220	36.160	25.177	13.180	-86.089	-64.108	11.676
1300	15.360	37.380	26.065	14.710	-85.844	-62.271	10.469
1400	15.490	38.520	26.913	16.250	-85.593	-60.468	9.439
1467	15.577	39.253	27.470	17.285	-85.424	-59.285	8.832
1467	15.577	39.253	27.470	17.285	-116.224	-59.285	8.832
1500	15.620	39.600	27.733	17.800	-116.011	-58.005	8.451
1600	15.760	40.610	28.504	19.370	-115.355	-54.155	7.397
1700	15.900	41.570	29.241	20.960	-114.683	-50.342	6.472
1800	16.030	42.480	29.952	22.550	-114.014	-46.579	5.655
1900	16.160	43.350	30.634	24.160	-113.327	-42.852	4.929
2000	16.300	44.180	31.290	25.780	-112.634	-39.159	4.279

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 553 K, second-order transition point of Yb; ΔH° = 0 kcal/mol.
1033 K, α - β transition point of Yb; ΔH° = 0.418 kcal/mol.
1097 K, melting point of Yb; ΔH° = 1.830 kcal./mol.
1467 K, boiling point of Yb; ΔH° = 30.800 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.600 + 1.350\times10^{-3}T$
$H^\circ - H^\circ_{298} = 13.600\times10^{-3}T + 0.675\times10^{-6}T^2 - 4.115$

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf^\circ = -89.804 + 9.318\times10^{-3}T - 5.321\times10^{-6}T^2 + 178.650T^{-1}$
$\Delta Gf^\circ = -89.804 - 9.318\times10^{-3}T\ln T + 5.321\times10^{-6}T^2 + 89.325T^{-1} + 81.422\times10^{-3}T$

553-1033 K: $\Delta Hf^\circ = -88.183 + 4.114\times10^{-3}T - 0.313\times10^{-6}T^2 + 26.650T^{-1}$
$\Delta Gf^\circ = -88.183 - 4.114\times10^{-3}T\ln T + 0.313\times10^{-6}T^2 + 13.325T^{-1} + 48.643\times10^{-3}T$

1033-1097 K: $\Delta Hf^\circ = -86.828 + 1.701\times10^{-3}T + 0.381\times10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf^\circ = -86.828 - 1.701\times10^{-3}T\ln T - 0.381\times10^{-6}T^2 + 1.975T^{-1} + 31.319\times10^{-3}T$

1097-1467 K: $\Delta Hf^\circ = -88.498 + 1.555\times10^{-3}T + 0.381\times10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf^\circ = -88.498 - 1.555\times10^{-3}T\ln T - 0.381\times10^{-6}T^2 + 1.975T^{-1} + 31.819\times10^{-3}T$

1467-2000 K: $\Delta Hf^\circ = -124.899 + 5.374\times10^{-3}T + 0.381\times10^{-6}T^2 + 3.950T^{-1}$
$\Delta Gf^\circ = -124.899 - 5.374\times10^{-3}T\ln T - 0.381\times10^{-6}T^2 + 1.975T^{-1} + 84.469\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Brown (60). Other data are those estimated by Brown (59).

$YbO(g)$
Ytterbium Monoxide (ideal gas)
[Formation: $Yb(c,l,g) + 0.5O_2(g) = YbO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.540	60.023	60.023	0	-17.000	-23.327	17.099
300	7.550	60.070	60.023	.014	-17.004	-23.366	17.022
400	7.930	62.297	60.325	.789	-17.232	-25.452	13.906
500	8.200	64.096	60.904	1.596	-17.483	-27.476	12.009
553	8.301	64.928	61.251	2.034	-17.660	-28.526	11.274
600	8.390	65.609	61.566	2.426	-17.781	-29.445	10.725
700	8.510	66.911	62.238	3.271	-18.042	-31.366	9.793
800	8.600	68.055	62.896	4.127	-18.316	-33.256	9.085
900	8.670	69.072	63.526	4.991	-18.604	-35.103	8.524
1000	8.710	69.988	64.128	5.860	-18.904	-36.927	8.070
1033	8.723	70.271	64.320	6.148	-19.008	-37.517	7.937
1033	8.723	70.271	64.320	6.148	-19.426	-37.517	7.937
1097	8.749	70.797	64.682	6.708	-19.688	-38.625	7.695
1097	8.749	70.797	64.682	6.708	-21.518	-38.625	7.695
1100	8.750	70.821	64.699	6.734	-21.529	-38.674	7.684
1200	8.780	71.583	65.241	7.610	-21.957	-40.219	7.325
1300	8.800	72.287	65.757	8.489	-22.385	-41.716	7.013
1400	8.820	72.941	66.247	9.371	-22.813	-43.190	6.742
1467	8.833	73.352	66.561	9.962	-23.102	-44.156	6.578
1467	8.833	73.352	66.561	9.962	-53.902	-44.156	6.578
1500	8.840	73.549	66.713	10.254	-53.919	-43.935	6.401
1600	8.850	74.120	67.159	11.138	-53.970	-43.270	5.910
1700	8.860	74.657	67.584	12.024	-54.021	-42.597	5.476
1800	8.870	75.163	67.991	12.910	-54.076	-41.922	5.090
1900	8.880	75.644	68.382	13.797	-54.133	-41.250	4.745
2000	8.880	76.099	68.757	14.685	-54.191	-40.569	4.433

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 553 K, second-order transition point of Yb; ΔH° = 0 kcal/mol.
1033 K, α - β transition point of Yb; ΔH° = 0.418 kcal/mol.
1097 K, melting point of Yb; ΔH° = 1.830 kcal./mol.
1467 K, boiling point of Yb; ΔH° = 30.800 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.433 + 0.312\times10^{-3}T - 0.876\times10^{5}T^{-2}$
$H°- H°_{298} = 8.433\times10^{-3}T + 0.156\times10^{-6}T^{2} + 0.876\times10^{2}T^{-1} - 2.822$

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf° = -18.420 + 3.794\times10^{-3}T - 5.797\times10^{-6}T^{2} + 239.700T^{-1}$
$\Delta Gf° = -18.420 - 3.794\times10^{-3}T\ln T + 5.797\times10^{-6}T^{2} + 119.850T^{-1} + 2.081\times10^{-3}T$
553-1033 K: $\Delta Hf° = -16.799 - 1.410\times10^{-3}T - 0.789\times10^{-6}T^{2} + 87.700T^{-1}$
$\Delta Gf° = -16.799 + 1.410\times10^{-3}T\ln T + 0.789\times10^{-6}T^{2} + 43.850T^{-1} - 30.697\times10^{-3}T$
1033-1097 K: $\Delta Hf° = -15.444 - 3.822\times10^{-3}T - 0.095\times10^{-6}T^{2} + 65.000T^{-1}$
$\Delta Gf° = -15.444 + 3.822\times10^{-3}T\ln T + 0.095\times10^{-6}T^{2} + 32.500T^{-1} - 48.021\times10^{-3}T$
1097-1467 K: $\Delta Hf° = -17.113 - 3.968\times10^{-3}T - 0.095\times10^{-6}T^{2} + 65.000T^{-1}$
$\Delta Gf° = -17.113 + 3.968\times10^{-3}T\ln T + 0.095\times10^{-6}T^{2} + 32.500T^{-1} - 47.521\times10^{-3}T$
1467-2000 K: $\Delta Hf° = -53.514 - 0.150\times10^{-3}T - 0.095\times10^{-6}T^{2} + 65.000T^{-1}$
$\Delta Gf° = -53.514 + 0.150\times10^{-3}T\ln T + 0.095\times10^{-6}T^{2} + 32.500T^{-1} + 5.129\times10^{-3}T$

Source: Data from Pedley (396) who estimated all except enthalpy of formation at 298 K.

$ZnCO_3$(c)
Zinc Carbonate, Smithsonite
[Formation: $Zn(c) + C(c) + 1.5O_2(g) = ZnCO_3(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.050	19.700	19.700	0	-194.810	-175.392	128.564
300*	19.200	19.820	19.703	.035	-194.809	-175.272	127.684
400	22.500	25.790	20.490	2.120	-194.652	-168.774	92.213
500	25.800	31.170	22.100	4.535	-194.290	-162.345	70.960

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp° = 10.190 + 31.510 \times 10^{-3}T - 0.442 \times 10^{5}T^{-2}$

$H°- H°_{298} = 10.190 \times 10^{-3}T + 15.755 \times 10^{-6}T^{2} + 0.442 \times 10^{2}T^{-1} - 4.587$

Formation equations (kcal/mol):

298.15-500 K: $\Delta Hf° = -192.572 - 9.272 \times 10^{-3}T + 12.842 \times 10^{-6}T^{2} - 183.300T^{-1}$

$\Delta Gf° = -192.572 + 9.272 \times 10^{-3}T\ln T - 12.842 \times 10^{-6}T^{2} - 91.650T^{-1} + 9.656 \times 10^{-3}T$

Source: Data from Chang (74) who estimated all above 298 K.

$ZnFe_2O_4(c)$
Zinc Ferrite
[Formation: $Zn(c,l) + 2Fe(c) + 2O_2(g) = ZnFe_2O_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^\circ_{298})/T$	$H°-H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	32.990	36.010	36.010	0	-277.600	-252.260	184.909
300	33.106	36.214	36.011	.061	-277.598	-252.102	183.654
400	37.176	46.376	37.368	3.603	-277.346	-243.635	133.114
500	39.322	54.920	40.048	7.436	-276.979	-235.250	102.826
600	40.846	62.230	43.150	11.448	-276.617	-226.936	82.660
692.73	42.024	68.185	46.111	15.291	-276.330	-219.282	69.180
692.73	42.024	68.185	46.111	15.291	-278.080	-219.282	69.180
700	42.116	68.624	46.343	15.597	-278.064	-218.665	68.269
800	43.267	74.324	49.490	19.867	-277.870	-210.196	57.422
900	44.354	79.483	52.541	24.248	-277.791	-201.743	48.989
1000	45.406	84.211	55.474	28.737	-277.978	-193.288	42.243

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 38.250 + 7.610\times10^{-3}T - 6.692\times10^{5}T^{-2}$

$H°-H^\circ_{298} = 38.250\times10^{-3}T + 3.805\times10^{-6}T^{2} + 6.692\times10^{2}T^{-1} - 13.987$

Formation equations (kcal/mol):

298.15-692.73 K: $\Delta Hf° = -285.867 + 19.133\times10^{-3}T - 10.735\times10^{-6}T^{2} + 1048.400T^{-1}$

$\Delta Gf° = -285.867 - 19.133\times10^{-3}T\ln T + 10.735\times10^{-6}T^{2} + 524.200T^{-1} + 212.631\times10^{-3}T$

692.73-1000 K: $\Delta Hf° = -286.603 + 16.732\times10^{-3}T - 9.343\times10^{-6}T^{2} + 1035.800T^{-1}$

$\Delta Gf° = -286.603 - 16.732\times10^{-3}T\ln T + 9.343\times10^{-6}T^{2} + 517.900T^{-1} + 198.967\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Khomyakov (254). Low-temperature heat capacities and entropy at 298 K from Westrum (528). High-temperature data based on Carling (68).

$Zn_3N_2(c)$
Trizinc Dinitride
[Formation: $3Zn(c,l) + N_2(g) = Zn_3N_2(c)$]

T,K	cal/mol•K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H^{\circ}_{298})/T$	$H°-H^{\circ}_{298}$	ΔHf°	ΔGf°	
298.15*	26.130	26.000	26.000	0	-5.400	9.394	-6.886
300	26.170	26.160	26.000	.050	-5.396	9.489	-6.913
400	28.250	33.980	27.055	2.770	-5.227	14.426	-7.882
500	30.330	40.500	29.100	5.700	-4.920	19.310	-8.440
600	32.410	46.220	31.503	8.830	-4.501	24.107	-8.781
692.73	34.339	51.011	33.789	11.930	-4.010	28.493	-8.989
692.73	34.339	51.011	33.789	11.930	-9.260	28.493	-8.989
700	34.490	51.370	33.970	12.180	-9.228	28.890	-9.020

*Data except enthalpy of formation at 298 K estimated.

Phase change: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp° = 19.930 + 20.800\times10^{-3}T$

$H°-H^{\circ}_{298} = 19.930\times10^{-3}T + 10.400\times10^{-6}T^2 - 6.867$

Formation equations (kcal/mol):

298.15-692.73 K: $\Delta Hf° = -5.492 - 1.884\times10^{-3}T + 5.635\times10^{-6}T^2 + 45.700T^{-1}$

$\Delta Gf° = -5.492 + 1.884\times10^{-3}T\ln T - 5.635\times10^{-6}T^2 + 22.850T^{-1} + 40.619\times10^{-3}T$

692.73- 700 K: $\Delta Hf° = -7.702 - 9.087\times10^{-3}T + 9.811\times10^{-6}T^2 + 7.900T^{-1}$

$\Delta Gf° = -7.702 + 9.087\times10^{-3}T\ln T - 9.811\times10^{-6}T^2 + 3.950T^{-1} - 0.371\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Entropy at 298 K estimated. High-temperature data based on heat capacities estimated by Kelley (243).

ZnO(g)
Zinc Monoxide (ideal gas)
[Formation: $Zn(c,l,g) + 0.5O_2(g) = ZnO(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.820	53.681	53.681	0	26.000	20.267	-14.856
300	7.830	53.729	53.682	.014	25.997	20.232	-14.738
400	8.190	56.035	53.993	.817	25.826	18.337	-10.018
500	8.410	57.889	54.593	1.648	25.652	16.483	-7.205
600	8.550	59.436	55.274	2.497	25.458	14.668	-5.343
692.73	8.643	60.672	55.916	3.294	25.249	13.012	-4.105
692.73	8.643	60.672	55.916	3.294	23.499	13.012	-4.105
700	8.650	60.762	55.966	3.357	23.479	12.903	-4.028
800	8.710	61.921	56.640	4.225	23.198	11.411	-3.117
900	8.760	62.950	57.284	5.099	22.915	9.955	-2.417
1000	8.790	63.874	57.898	5.976	22.628	8.530	-1.864
1100	8.810	64.713	58.480	6.856	22.338	7.134	-1.417
1180	8.826	65.333	58.924	7.562	22.106	6.040	-1.119
1180	8.826	65.333	58.924	7.562	-5.459	6.040	-1.119
1200	8.830	65.481	59.032	7.739	-5.468	6.234	-1.135
1300	8.850	66.189	59.556	8.623	-5.508	7.209	-1.212
1400	8.860	66.845	60.053	9.509	-5.552	8.190	-1.279
1500	8.870	67.457	60.527	10.395	-5.597	9.171	-1.336
1600	8.880	68.030	60.978	11.283	-5.645	10.157	-1.387
1700	8.890	68.568	61.409	12.171	-5.695	11.147	-1.433
1800	8.890	69.077	61.821	13.060	-5.747	12.138	-1.474
1900	8.900	69.557	62.215	13.950	-5.801	13.135	-1.511
2000	8.900	70.014	62.594	14.840	-5.857	14.131	-1.544

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.671 + 0.166\times10^{-3}T - 0.801\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 8.671\times10^{-3}T + 0.083\times10^{-6}T^2 + 0.801\times10^{2}T^{-1} - 2.861$

Formation equations (kcal/mol):

298.15-692.73 K: $\Delta Hf^\circ = 25.916 - 0.043\times10^{-3}T - 1.561\times10^{-6}T^2 + 70.100T^{-1}$
$\Delta Gf^\circ = 25.916 + 0.043\times10^{-3}T\ln T + 1.561\times10^{-6}T^2 + 35.050T^{-1} - 20.053\times10^{-3}T$
692.73-1180 K: $\Delta Hf^\circ = 25.180 - 2.444\times10^{-3}T - 0.168\times10^{-6}T^2 + 57.500T^{-1}$
$\Delta Gf^\circ = 25.180 + 2.444\times10^{-3}T\ln T + 0.168\times10^{-6}T^2 + 28.750T^{-1} - 33.716\times10^{-3}T$
1180-2000 K: $\Delta Hf^\circ = -5.373 + 0.088\times10^{-3}T - 0.168\times10^{-6}T^2 + 57.500T^{-1}$
$\Delta Gf^\circ = -5.373 - 0.088\times10^{-3}T\ln T + 0.168\times10^{-6}T^2 + 28.750T^{-1} + 10.086\times10^{-3}T$

Source: Data from Pedley (396).

$ZnO \cdot 2ZnSO_4(c)$
Zinc Oxysulfate
[Reaction: $3Zn(c,l,g) + 4.5O_2(g) + S_2(g) = ZnO \cdot 2ZnSO_4(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	$Cp°$	$S°$	$-(G°-H°_{298})/T$	$H°-H°_{298}$	$\Delta Hr°$	$\Delta Gr°$	
298.15	59.000	69.450	69.450	0	-581.020	-510.827	374.441
300	58.696	69.814	69.451	.109	-581.016	-510.389	371.813
400	66.536	87.744	71.834	6.364	-580.608	-486.888	266.020
500	71.408	103.159	76.597	13.281	-579.728	-463.553	202.616
600	74.644	116.481	82.161	20.592	-578.661	-440.417	160.420
692.73	76.927	127.375	87.498	27.624	-577.605	-419.136	132.232
692.73	76.927	127.375	87.498	27.624	-582.855	-419.136	132.232
700	77.106	128.179	87.916	28.184	-582.780	-417.417	130.322
800	79.157	138.612	93.612	36.000	-581.677	-393.869	107.599
900	80.968	148.042	99.144	44.008	-580.461	-370.466	89.960
1000	82.630	156.660	104.472	52.188	-579.140	-347.205	75.881
1100	84.195	164.609	109.582	60.530	-577.719	-324.076	64.387
1180	85.394	170.562	113.516	67.314	-576.505	-305.662	56.612
1180	85.394	170.562	113.516	67.314	-659.200	-305.662	56.612
1200	85.694	172.000	114.479	69.025	-658.737	-299.679	54.578

Phase changes: 692.73 K, melting point of Zn; $\Delta H° = 1.750$ kcal/mol.
1180 K, boiling point of Zn; $\Delta H° = 27.565$ Kcal/mol.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 67.054 + 17.172\text{x}10^{-3}T - 11.711\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 67.054\text{x}10^{-3}T + 8.586\text{x}10^{-6}T^{2} + 11.711\text{x}10^{2}T^{-1} - 24.683$

Reaction equations (kcal/mol):

298.15-692.73 K: $\Delta Hr° = -587.569 + 10.879\text{x}10^{-3}T + 1.827\text{x}10^{-6}T^{2} + 937.200T^{-1}$
$\Delta Gr° = -587.569 - 10.879\text{x}10^{-3}T\ln T - 1.827\text{x}10^{-6}T^{2} + 468.600T^{-1} + 314.652\text{x}10^{-3}T$
692.73-1180 K: $\Delta Hr° = -589.779 + 3.676\text{x}10^{-3}T + 6.003\text{x}10^{-6}T^{2} + 899.400T^{-1}$
$\Delta Gr° = -589.779 - 3.676\text{x}10^{-3}T\ln T - 6.003\text{x}10^{-6}T^{2} + 449.700T^{-1} + 273.662\text{x}10^{-3}T$
1180-1200 K: $\Delta Hr° = -681.437 + 11.272\text{x}10^{-3}T + 6.003\text{x}10^{-6}T^{2} + 899.400T^{-1}$
$\Delta Gr° = -681.437 - 11.272\text{x}10^{-3}T\ln T - 6.003\text{x}10^{-6}T^{2} + 449.700T^{-1} + 405.067\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from DeKock (112). Other data from Beyer (38).

$ZnSO_4(c)$
Zinc Sulfate
[Reaction: $Zn(c,l,g) + 2O_2(g) + 0.5S_2(g) = ZnSO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	23.680	26.430	26.430	0	-249.615	-217.181	159.196
300	23.746	26.577	26.430	.044	-249.615	-216.979	158.067
400	26.878	33.859	27.402	2.583	-249.513	-206.110	112.612
500	29.506	40.144	29.336	5.404	-249.207	-195.290	85.360
600	31.945	45.741	31.611	8.478	-248.734	-184.548	67.221
692.73	34.124	50.486	33.825	11.541	-248.156	-174.672	55.107
692.73	34.124	50.486	33.825	11.541	-249.906	-174.672	55.107
700	34.295	50.843	34.000	11.790	-249.858	-173.882	54.288
800	36.597	55.573	36.404	15.335	-249.094	-163.080	44.551
900	38.871	60.015	38.783	19.109	-248.139	-152.383	37.003
1000	41.128	64.227	41.118	23.109	-246.986	-141.804	30.991
1015	41.466	64.842	41.285	23.910	-246.615	-140.046	30.154
1015	34.700	69.640	41.285	28.780	-241.745	-140.046	30.154
1100	34.700	72.431	43.586	31.729	-241.242	-131.549	26.136
1180	34.700	74.867	45.625	34.505	-240.781	-123.584	22.889
1180	34.700	74.867	45.625	34.505	-268.346	-123.584	22.889
1200	34.700	75.450	46.117	35.199	-268.184	-121.134	22.061

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1015 K, α - β transition point of $ZnSO_4$; ΔH° = 4.870 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1015 K: $Cp° = 17.737 + 24.380\times10^{-3}T - 1.178\times10^{5}T^{-2}$
$H°-H°_{298} = 17.737\times10^{-3}T + 12.190\times10^{-6}T^{2} + 1.178\times10^{2}T^{-1} - 6.767$
1015-1200 K: $Cp° = 34.989 - 0.190\times10^{-3}T - 0.991\times10^{5}T^{-2}$
$H°-H°_{298} = 34.989\times10^{-3}T - 0.095\times10^{-6}T^{2} + 0.991\times10^{2}T^{-1} - 6.734$

Reaction equations (kcal/mol):

298.15-692.73 K: $\Delta Hr° = -248.704 - 5.994\times10^{-3}T + 9.632\times10^{-6}T^{2} + 5.850T^{-1}$
$\Delta Gr° = -248.704 + 5.994\times10^{-3}T\ln T - 9.632\times10^{-6}T^{2} + 2.925T^{-1} + 74.417\times10^{-3}T$
692.73-1015 K: $\Delta Hr° = -249.440 - 8.394\times10^{-3}T + 11.024\times10^{-6}T^{2} - 6.750T^{-1}$
$\Delta Gr° = -249.440 + 8.394\times10^{-3}T\ln T - 11.024\times10^{-6}T^{2} - 3.375T^{-1} + 60.754\times10^{-3}T$
1015-1180 K: $\Delta Hr° = -249.406 + 8.858\times10^{-3}T - 1.261\times10^{-6}T^{2} - 25.450T^{-1}$
$\Delta Gr° = -249.406 - 8.858\times10^{-3}T\ln T + 1.261\times10^{-6}T^{2} - 12.725T^{-1} + 167.690\times10^{-3}T$
1180-1200 K: $\Delta Hr° = -279.959 + 11.389\times10^{-3}T - 1.261\times10^{-6}T^{2} - 25.450T^{-1}$
$\Delta Gr° = -279.959 - 11.389\times10^{-3}T\ln T + 1.261\times10^{-6}T^{2} - 12.725T^{-1} + 211.491\times10^{-3}T$

Source: Data from DeKock (112).

$ZnSO_4 \cdot H_2O(c)$
Zinc Sulfate Monohydrate
[Reaction: $Zn(c) + H_2(g) + 2.5O_2(g) + 0.5S_2(g) = ZnSO_4 \cdot H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G° - H°_{298})/T$	$H° - H°_{298}$	ΔHr°	ΔGr°	
298.15	36.153	33.100	33.100	0	-327.205	-280.150	205.353
300*	36.319	33.324	33.101	.067	-327.202	-279.857	203.873
350	40.819	39.261	33.561	1.995	-327.005	-271.980	169.830
400	45.320	45.005	34.632	4.149	-326.606	-264.144	144.320
450	49.820	50.603	36.099	6.527	-326.005	-256.370	124.509
500	54.320	56.085	37.823	9.131	-325.203	-248.673	108.694
550	58.820	61.473	39.729	11.959	-324.202	-241.068	95.790

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 8.954 + 90.632\text{x}10^{-3}T + 0.158\text{x}10^{5}T^{-2}$

$H° - H°_{298} = 8.954\text{x}10^{-3}T + 45.316\text{x}10^{-6}T^{2} - 0.158\text{x}10^{2}T^{-1} - 6.645$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -323.089 - 24.848\text{x}10^{-3}T + 42.088\text{x}10^{-6}T^{2} - 133.850T^{-1}$

$\Delta Gr° = -323.089 + 24.848\text{x}10^{-3}T\ln T - 42.088\text{x}10^{-6}T^{2} - 66.925T^{-1} + 15.748\text{x}10^{-3}T$

Source: Data from DeKock (112) who estimated all above 298 K.

$ZnSO_4 \cdot 6H_2O(c)$
Zinc Sulfate Hexahydrate
[Reaction: $Zn(c) + 6H_2(g) + 5O_2(g) + 0.5S_2(g) = ZnSO_4 \cdot 6H_2O(c)$]

T,K	cal/mol•K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	84.994	86.900	86.900	0	-679.255	-565.192	414.291
300*	85.456	87.427	86.900	.158	-679.258	-564.483	411.220
333.4	93.988	96.887	87.430	3.153	-679.160	-551.708	361.650
350	98.362	101.559	87.988	4.750	-679.010	-545.364	340.537
400	112.072	115.580	90.563	10.007	-678.140	-526.324	287.566
450	126.586	129.610	94.121	15.970	-676.609	-507.433	246.440
500	141.904	143.733	98.375	22.679	-674.370	-488.748	213.629
550	158.026	158.008	103.146	30.174	-671.387	-470.325	186.887

*Data above 298 K except dissociation temperature estimated.

Phase change: 333.4 K, dissociation point of $ZnSO_4 \cdot 6H_2O$; to $ZnSO_4 \cdot H_2O$ and saturated solution.

Heat capacity (cal/mol•K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp^\circ = -25.156 + 324.840\times10^{-3}T + 11.822\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -25.156\times10^{-3}T + 162.420\times10^{-6}T^{2} - 11.822\times10^{2}T^{-1} - 2.973$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr^\circ = -656.053 - 109.313\times10^{-3}T + 155.839\times10^{-6}T^{2} - 1330.750T^{-1}$

$\Delta Gr^\circ = -656.053 + 109.313\times10^{-3}T\ln T - 155.839\times10^{-6}T^{2} - 665.375T^{-1} - 264.119\times10^{-3}T$

Source: Data from DeKock (112) who estimated all above 298 K except dissociation temperature.

$ZnSO_4 \cdot 7H_2O(c)$
Zinc Sulfate Heptahydrate
[Reaction: $Zn(c) + 7H_2(g) + 5.5O_2(g) + 0.5S_2(g) = ZnSO_4 \cdot 7H_2O(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	91.144	92.900	92.900	0	-750.905	-622.021	455.948
300	91.620	93.465	92.902	.169	-750.917	-621.220	452.553
311.27	94.590	96.898	92.982	1.219	-750.959	-616.347	432.746
350	103.820	108.512	94.063	5.057	-750.895	-599.598	374.401
400	115.631	123.150	96.788	10.545	-750.320	-578.016	315.809
450	127.078	137.434	100.514	16.614	-749.214	-556.540	270.289
500	138.163	151.400	104.906	23.247	-747.586	-535.213	233.939
550	148.885	165.074	109.756	30.425	-745.456	-514.075	204.272

Phase change: 311.27 K, dissociation point of $ZnSO_4 \cdot 7H_2O$ to $ZnSO_4 \cdot 6H_2O$ and saturated solution; ΔH° = 4.017 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $Cp° = 33.453 + 213.584 \times 10^{-3}T - 5.285 \times 10^{5}T^{-2}$

$H° - H°_{298} = 33.453 \times 10^{-3}T + 106.792 \times 10^{-6}T^{2} + 5.285 \times 10^{2}T^{-1} - 21.240$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta Hr° = -742.887 - 60.774 \times 10^{-3}T + 99.540 \times 10^{-6}T^{2} + 373.850T^{-1}$

$\Delta Gr° = -742.887 + 60.774 \times 10^{-3}T\ln T - 99.540 \times 10^{-6}T^{2} + 186.925T^{-1} + 86.695 \times 10^{-3}T$

Source: Data from DeKock (112).

$ZnSe(g)$
Zinc Selenide (ideal gas)
[Reaction: $Zn(c,l,g) + 0.5Se_2(g) = ZnSe(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	8.697	59.840	59.840	0	38.480	32.281	-23.663
300	8.700	59.894	59.841	.016	38.476	32.243	-23.489
400	8.804	62.413	60.183	.892	38.236	30.201	-16.501
500	8.852	64.383	60.833	1.775	37.976	28.222	-12.336
600	8.878	66.000	61.563	2.662	37.691	26.297	-9.579
692.73	8.892	67.276	62.245	3.485	37.401	24.556	-7.747
692.73	8.892	67.276	62.245	3.485	35.651	24.556	-7.747
700	8.893	67.369	62.298	3.550	35.624	24.439	-7.630
800	8.904	68.558	63.008	4.440	35.260	22.868	-6.247
900	8.911	69.607	63.684	5.331	34.899	21.340	-5.182
1000	8.916	70.546	64.324	6.222	34.541	19.851	-4.338
1100	8.919	71.396	64.929	7.114	34.186	18.400	-3.656
1180	8.921	72.022	65.389	7.828	33.904	17.266	-3.198
1180	8.921	72.022	65.389	7.828	6.339	17.266	-3.198
1200	8.922	72.172	65.500	8.006	6.319	17.450	-3.178
1300	8.924	72.886	66.041	8.898	6.222	18.382	-3.090
1400	8.926	73.548	66.554	9.791	6.130	19.319	-3.016
1500	8.927	74.163	67.041	10.683	6.039	20.264	-2.952
1600	8.929	74.740	67.505	11.576	5.952	21.212	-2.897

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp^\circ = 8.935 + 0.002\mathrm{x}10^{-3}T - 0.212\mathrm{x}10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.935\mathrm{x}10^{-3}T + 0.001\mathrm{x}10^{-6}T^{2} + 0.212\mathrm{x}10^{2}T^{-1} - 2.735$

Reaction equations (kcal/mol):

298.15-692.73 K: $\Delta Hr^\circ = 39.023 - 1.496\mathrm{x}10^{-3}T - 1.232\mathrm{x}10^{-6}T^{2} + 3.850T^{-1}$

$\Delta Gr^\circ = 39.023 + 1.496\mathrm{x}10^{-3}T\ln T + 1.232\mathrm{x}10^{-6}T^{2} + 1.925T^{-1} - 31.522\mathrm{x}10^{-3}T$

692.73-1180 K: $\Delta Hr^\circ = 38.286 - 3.897\mathrm{x}10^{-3}T + 0.161\mathrm{x}10^{-6}T^{2} - 8.750T^{-1}$

$\Delta Gr^\circ = 38.286 + 3.897\mathrm{x}10^{-3}T\ln T - 0.161\mathrm{x}10^{-6}T^{2} - 4.375T^{-1} - 45.186\mathrm{x}10^{-3}T$

1180-1600 K: $\Delta Hr^\circ = 7.733 - 1.365\mathrm{x}10^{-3}T + 0.161\mathrm{x}10^{-6}T^{2} - 8.750T^{-1}$

$\Delta Gr^\circ = 7.733 + 1.365\mathrm{x}10^{-3}T\ln T - 0.161\mathrm{x}10^{-6}T^{2} - 4.375T^{-1} - 1.384\mathrm{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K based on DeMaria (115). Other data from Pashinkin (393) who estimated molecular constants.

$Zn_2SiO_4(c)$
Zinc Silicate
[Formation: $2Zn(c,l,g) + Si(c) + 2O_2(g) = Zn_2SiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	29.480	31.400	31.400	0	-391.190	-364.055	266.856
300	29.640	31.580	31.413	.050	-391.197	-363.890	265.090
400	35.030	40.930	32.630	3.320	-391.090	-354.786	193.844
500	38.160	49.110	35.130	6.990	-390.708	-345.751	151.126
600	40.340	56.270	38.070	10.920	-390.192	-336.808	122.681
692.73	41.907	62.182	40.911	14.735	-389.656	-328.603	103.670
692.73	41.907	62.182	40.911	14.735	-393.156	-328.603	103.670
700	42.030	62.620	41.134	15.040	-393.119	-327.925	102.382
800	43.410	68.320	44.182	19.310	-392.550	-318.649	87.050
900	44.570	73.510	47.166	23.710	-391.898	-309.458	75.146
1000	45.570	78.260	50.040	28.220	-391.170	-300.328	65.636
1100	46.430	82.640	52.804	32.820	-390.385	-291.284	57.872
1180	47.006	85.919	54.937	36.558	-389.717	-284.092	52.617
1180	47.006	85.919	54.937	36.558	-444.847	-284.092	52.617
1200	47.150	86.710	55.460	37.500	-444.575	-281.373	51.244
1300	47.770	90.510	58.010	42.250	-443.181	-267.829	45.026
1400	48.270	94.070	60.463	47.050	-441.760	-254.392	39.712
1500	48.670	97.410	62.810	51.900	-440.307	-241.065	35.123
1600	48.970	100.570	65.083	56.780	-438.843	-227.848	31.122

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K:
$$Cp^\circ = 38.041 + 8.150\times10^{-3}T - 9.770\times10^{5}T^{-2}$$
$$H^\circ - H^\circ_{298} = 38.041\times10^{-3}T + 4.075\times10^{-6}T^{2} + 9.770\times10^{2}T^{-1} - 14.981$$

Formation equations (kcal/mol):

298.15-692.73 K:
$$\Delta Hf^\circ = -396.209 + 7.704\times10^{-3}T - 0.066\times10^{-6}T^{2} + 813.300T^{-1}$$
$$\Delta Gf^\circ = -396.209 - 7.704\times10^{-3}T\ln T + 0.066\times10^{-6}T^{2} + 406.650T^{-1} + 147.143\times10^{-3}T$$

692.73-1180 K:
$$\Delta Hf^\circ = -397.682 + 2.902\times10^{-3}T + 2.718\times10^{-6}T^{2} + 788.100T^{-1}$$
$$\Delta Gf^\circ = -397.682 - 2.902\times10^{-3}T\ln T - 2.718\times10^{-6}T^{2} + 394.050T^{-1} + 119.817\times10^{-3}T$$

1180-1600 K:
$$\Delta Hf^\circ = -458.788 + 7.966\times10^{-3}T + 2.718\times10^{-6}T^{2} + 788.100T^{-1}$$
$$\Delta Gf^\circ = -458.788 - 7.966\times10^{-3}T\ln T - 2.718\times10^{-6}T^{2} + 394.050T^{-1} + 207.420\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from Todd (494). High-temperature data based on Egorov (138).

ZnTe(c)
Zinc Telluride
[Reaction: Zn(c,l,g) + 0.5Te$_2$(g) = ZnTe(c)]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H°$_{298}$)/T	H°- H°$_{298}$	ΔHr°	ΔGr°	
298.15	11.880	18.600	18.600	0	-47.665	-41.021	30.069
300	11.890	18.670	18.600	.022	-47.662	-40.979	29.853
400	12.330	22.160	19.075	1.234	-47.508	-38.776	21.186
500	12.780	24.960	19.980	2.490	-47.340	-36.612	16.003
600	13.230	27.330	21.013	3.790	-47.162	-34.481	12.560
692.73	13.647	29.257	21.988	5.036	-46.992	-32.535	10.264
692.73	13.647	29.257	21.988	5.036	-48.742	-32.535	10.264
700	13.680	29.400	22.064	5.135	-48.732	-32.365	10.105
800	14.120	31.260	23.104	6.525	-48.565	-30.042	8.207
900	14.570	32.950	24.106	7.960	-48.360	-27.740	6.736
1000	15.020	34.510	25.070	9.440	-48.119	-25.463	5.565
1100	15.470	35.960	25.993	10.964	-47.842	-23.206	4.611
1180	15.830	37.053	26.701	12.215	-47.593	-21.413	3.966
1180	15.830	37.053	26.701	12.215	-75.158	-21.413	3.966
1200	15.920	37.320	26.876	12.533	-75.043	-20.505	3.734
1300	16.360	38.610	27.728	14.147	-74.438	-15.983	2.687

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp° = 10.577 + 4.436\times10^{-3}T - 0.018\times10^{5}T^{-2}$
$H° - H°_{298} = 10.577\times10^{-3}T + 2.218\times10^{-6}T^{2} + 0.018\times10^{2}T^{-1} - 3.357$

Reaction equations (kcal/mol):

298.15-692.73 K: $\Delta Hr° = -48.071 + 1.178\times10^{-3}T + 0.529\times10^{-6}T^{2} + 2.300T^{-1}$
$\Delta Gr° = -48.071 - 1.178\times10^{-3}T\ln T - 0.529\times10^{-6}T^{2} + 1.150T^{-1} + 30.507\times10^{-3}T$
692.73-1180 K: $\Delta Hr° = -48.808 - 1.223\times10^{-3}T + 1.921\times10^{-6}T^{2} - 10.300T^{-1}$
$\Delta Gr° = -48.808 + 1.223\times10^{-3}T\ln T - 1.921\times10^{-6}T^{2} - 5.150T^{-1} + 16.843\times10^{-3}T$
1180-1300 K: $\Delta Hr° = -79.360 + 1.309\times10^{-3}T + 1.921\times10^{-6}T^{2} - 10.300T^{-1}$
$\Delta Gr° = -79.360 - 1.309\times10^{-3}T\ln T - 1.921\times10^{-6}T^{2} - 5.150T^{-1} + 60.645\times10^{-3}T$

Source: Data from Mills (332).

$ZnTe(g)$
Zinc Telluride (ideal gas)
[Reaction: $Zn(c,l,g) + 0.5Te_2g) = ZnTe(g)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	8.745	61.750	61.750	0	40.835	34.614	-25.372
300	8.748	61.804	61.751	.016	40.832	34.575	-25.188
400	8.825	64.333	62.096	.895	40.653	32.516	-17.766
500	8.861	66.307	62.747	1.780	40.450	30.505	-13.334
600	8.881	67.924	63.479	2.667	40.215	28.540	-10.395
692.73	8.892	69.201	64.161	3.491	39.964	26.750	-8.439
692.73	8.892	69.201	64.161	3.491	38.214	26.750	-8.439
700	8.893	69.294	64.214	3.556	38.189	26.630	-8.314
800	8.900	70.482	64.926	4.445	37.855	25.000	-6.830
900	8.905	71.531	65.602	5.336	37.516	23.413	-5.685
1000	8.909	72.469	66.242	6.227	37.168	21.865	-4.779
1100	8.912	73.318	66.847	7.118	36.813	20.354	-4.044
1180	8.914	73.944	67.308	7.831	36.522	19.170	-3.551
1180	8.914	73.944	67.308	7.831	8.957	19.170	-3.551
1200	8.914	74.094	67.420	8.009	8.933	19.342	-3.523
1300	8.916	74.807	67.961	8.900	8.815	20.213	-3.398
1400	8.917	75.468	68.474	9.792	8.689	21.095	-3.293
1500	8.918	76.083	68.960	10.684	8.562	21.984	-3.203
1600	8.919	76.659	69.424	11.576	8.435	22.880	-3.125

*Data estimated.

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp^\circ = 8.927 - 0.002\text{x}10^{-3}T - 0.162\text{x}10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 8.927\text{x}10^{-3}T - 0.001\text{x}10^{-6}T^{2} + 0.162\text{x}10^{2}T^{-1} - 2.716$

Reaction equations (kcal/mol):

298.15-692.73 K: $\Delta Hr^\circ = 41.070 - 0.472\text{x}10^{-3}T - 1.690\text{x}10^{-6}T^{2} + 16.700T^{-1}$
$\Delta Gr^\circ = 41.070 + 0.472\text{x}10^{-3}T\ln T + 1.690\text{x}10^{-6}T^{2} + 8.350T^{-1} - 24.936\text{x}10^{-3}T$
692.73-1180 K: $\Delta Hr^\circ = 40.333 - 2.873\text{x}10^{-3}T - 0.297\text{x}10^{-6}T^{2} + 4.100T^{-1}$
$\Delta Gr^\circ = 40.333 + 2.873\text{x}10^{-3}T\ln T + 0.297\text{x}10^{-6}T^{2} + 2.050T^{-1} - 38.600\text{x}10^{-3}T$
1180-1600 K: $\Delta Hr^\circ = 9.780 - 0.341\text{x}10^{-3}T - 0.297\text{x}10^{-6}T^{2} + 4.100T^{-1}$
$\Delta Gr^\circ = 9.780 + 0.341\text{x}10^{-3}T\ln T + 0.297\text{x}10^{-6}T^{2} + 2.050T^{-1} + 5.202\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K is that estimated by De Maria (115). Other data from Pashinkin (393) who estimated molecular constants.

$Zn_2TiO_4(c)$
Zinc Titanate
[Formation: $2Zn(c,l,g) + Ti(c,l) + 2O_2(g) = Zn_2TiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	32.820	34.200	34.200	0	-393.800	-366.659	268.765
300	32.916	34.403	34.200	.061	-393.798	-366.489	266.983
400	36.694	44.444	35.544	3.560	-393.571	-357.413	195.279
500	39.023	52.899	38.193	7.353	-393.163	-348.420	152.293
600	40.730	60.171	41.264	11.344	-392.678	-339.516	123.667
692.73	42.000	66.116	44.199	15.182	-392.209	-331.332	104.531
692.73	42.000	66.116	44.199	15.182	-395.709	-331.332	104.531
700	42.100	66.555	44.429	15.488	-395.679	-330.657	103.234
800	43.252	72.254	47.558	19.757	-395.219	-321.401	87.802
900	44.242	77.407	50.593	24.133	-394.709	-312.203	75.812
1000	45.100	82.114	53.513	28.601	-394.153	-303.065	66.234
1100	45.843	86.448	56.313	33.149	-393.566	-293.990	58.410
1156	46.201	88.734	57.828	35.727	-393.224	-288.919	54.621
1156	46.201	88.734	57.828	35.727	-394.241	-288.919	54.621
1180	46.354	89.685	58.467	36.838	-394.066	-286.735	53.106
1180	46.354	89.685	58.467	36.838	-449.196	-286.735	53.106
1200	46.482	90.465	58.993	37.766	-448.950	-283.986	51.720
1300	47.023	94.208	61.560	42.442	-447.701	-270.293	45.440
1400	47.469	97.710	64.019	47.168	-446.438	-256.692	40.071
1500	47.825	100.997	66.375	51.933	-445.167	-243.184	35.431
1600	48.091	104.093	68.637	56.730	-443.900	-229.761	31.383
1700	48.270	107.014	70.809	61.549	-442.645	-216.414	27.822
1800	48.362	109.776	72.898	66.381	-441.419	-203.142	24.665

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 38.916 + 6.400\times10^{-3}T - 7.115\times10^{5}T^{-2}$
$H°-H°_{298} = 38.916\times10^{-3}T + 3.200\times10^{-6}T^{2} + 7.115\times10^{2}T^{-1} - 14.274$

Formation equations (kcal/mol):

298.15-692.73 K: $\Delta Hf° = -398.384 + 8.781\times10^{-3}T - 1.713\times10^{-6}T^{2} + 631.500T^{-1}$
$\Delta Gf° = -398.384 - 8.781\times10^{-3}T\ln T + 1.713\times10^{-6}T^{2} + 315.750T^{-1} + 152.372\times10^{-3}T$
692.73-1156 K: $\Delta Hf° = -399.857 + 3.979\times10^{-3}T + 1.071\times10^{-6}T^{2} + 606.300T^{-1}$
$\Delta Gf° = -399.857 - 3.979\times10^{-3}T\ln T - 1.071\times10^{-6}T^{2} + 303.150T^{-1} + 125.045\times10^{-3}T$
1156-1180 K: $\Delta Hf° = -403.894 + 6.379\times10^{-3}T + 0.748\times10^{-6}T^{2} + 1389.200T^{-1}$
$\Delta Gf° = -403.894 - 6.379\times10^{-3}T\ln T - 0.748\times10^{-6}T^{2} + 694.600T^{-1} + 144.798\times10^{-3}T$
1180-1800 K: $\Delta Hf° = -464.999 + 11.443\times10^{-3}T + 0.748\times10^{-6}T^{2} + 1389.200T^{-1}$
$\Delta Gf° = -464.999 - 11.443\times10^{-3}T\ln T - 0.748\times10^{-6}T^{2} + 694.600T^{-1} + 232.401\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (513). Low-temperature heat capacities and entropy at 298 K from King (259). High-temperature data based on Bonnickson (52).

$ZnWO_4(c)$
Zinc Tungstate
[Formation: $Zn(c,l) + W(c) + 2O_2(g) = ZnWO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	27.440	28.510	28.510	0	-293.000	-266.986	195.704
300	27.530	28.680	28.510	.051	-292.997	-266.823	194.378
400	31.010	37.127	29.639	2.995	-292.682	-258.139	141.039
500	33.100	44.288	31.872	6.208	-292.177	-249.559	109.081
600*	34.500	50.455	34.467	9.593	-291.586	-241.094	87.817
692.73	35.399	55.481	36.949	12.837	-291.008	-233.331	73.613
692.73	35.399	55.481	36.949	12.837	-292.758	-233.331	73.613
700	35.470	55.851	37.144	13.095	-292.716	-232.707	72.653
800	36.100	60.631	39.787	16.675	-292.114	-224.180	61.242
900	36.440	64.905	42.345	20.304	-291.504	-215.720	52.383
1000	36.520	68.750	44.796	23.954	-290.903	-207.332	45.312

*Data estimated above 550 K.

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 32.358 + 6.010\times10^{-3}T - 5.965\times10^{5}T^{-2}$

$H°- H°_{298} = 32.358\times10^{-3}T + 3.005\times10^{-6}T^{2} + 5.965\times10^{2}T^{-1} - 11.915$

Formation equations (kcal/mol):

298.15-692.73 K: $\Delta Hf° = -296.773 + 6.984\times10^{-3}T + 0.236\times10^{-6}T^{2} + 497.700T^{-1}$

$\Delta Gf° = -296.773 - 6.984\times10^{-3}T\ln T - 0.236\times10^{-6}T^{2} + 248.850T^{-1} + 136.966\times10^{-3}T$

692.73-1000 K: $\Delta Hf° = -297.509 + 4.583\times10^{-3}T + 1.628\times10^{-6}T^{2} + 485.100T^{-1}$

$\Delta Gf° = -297.509 - 4.583\times10^{-3}T\ln T - 1.628\times10^{-6}T^{2} + 242.550T^{-1} + 123.303\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (514). Other data based on Landee (292).

$ZrB_2(c)$
Zirconium Diboride
[Formation: $Zr(c,l) + 2B(\beta,l) = ZrB_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	11.530	8.590	8.590	0	-78.000	-76.942	56.399
300	11.589	8.662	8.592	.021	-78.000	-76.933	56.045
400	13.744	12.328	9.076	1.301	-77.994	-76.583	41.843
500	14.970	15.538	10.054	2.742	-78.034	-76.221	33.316
600	15.729	18.338	11.206	4.279	-78.139	-75.855	27.630
700	16.259	20.804	12.405	5.879	-78.288	-75.461	23.560
800	16.661	23.002	13.595	7.526	-78.468	-75.043	20.501
900	16.991	24.984	14.752	9.209	-78.677	-74.602	18.116
1000	17.245	26.788	15.867	10.921	-78.916	-74.136	16.202
1100	17.489	28.443	16.937	12.657	-79.182	-73.658	14.634
1136	17.577	29.008	17.310	13.288	-79.284	-73.476	14.136
1136	17.577	29.008	17.310	13.288	-80.235	-73.476	14.136
1200	17.733	29.975	17.959	14.419	-80.331	-73.087	13.311
1300	17.977	31.404	18.939	16.204	-80.501	-72.471	12.183
1400	18.221	32.745	19.878	18.014	-80.689	-71.845	11.215
1500	18.465	34.011	20.779	19.848	-80.900	-71.200	10.374
1600	18.709	35.210	21.643	21.707	-81.132	-70.569	9.639
1700	18.953	36.352	22.476	23.590	-81.384	-69.901	8.986
1800	19.197	37.442	23.276	25.498	-81.655	-69.194	8.401
1900	19.441	38.486	24.050	27.429	-81.947	-68.491	7.878
2000	19.685	39.490	24.797	29.386	-82.257	-67.801	7.409
2100	19.929	40.456	25.520	31.366	-82.588	-67.048	6.978
2125	19.990	40.692	25.697	31.865	-82.673	-66.864	6.877
2125	19.990	40.692	25.697	31.865	-87.673	-66.864	6.877
2200	20.173	41.389	26.220	33.372	-87.912	-66.145	6.571
2300	20.417	42.291	26.899	35.401	-88.235	-65.125	6.188
2350	20.539	42.731	27.231	36.425	-88.397	-64.652	6.013
2350	20.539	42.731	27.231	36.425	-112.397	-64.652	6.013
2400	20.661	43.165	27.559	37.455	-112.517	-63.617	5.793
2500	20.905	44.013	28.200	39.533	-112.739	-61.607	5.386
2600*	21.149	44.838	28.824	41.636	-112.936	-59.527	5.004
2700	21.393	45.641	29.432	43.763	-113.109	-57.486	4.653
2800	21.637	46.423	30.025	45.915	-113.257	-55.437	4.327
2900	21.881	47.187	30.604	48.090	-113.382	-53.332	4.019
3000	22.125	47.933	31.169	50.291	-113.481	-51.285	3.736

*Data extrapolated above 2500 K.

Phase changes:
1136 K, α - β transtion point of Zr; ΔH° = 0.951 kcal/mol.
2125 K, melting point of Zr; ΔH° = 5.000 kcal/mol.
2350 K, melting point of B; ΔH° = 12.0 kcal/mol.
3323 K, melting point of ZrB_2; ΔH° = 24.9 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3323 K: $Cp° = 15.346 + 2.256\text{x}10^{-3}T - 3.965\text{x}10^{5}T^{-2}$
$H°-H°_{298} = 15.346\text{x}10^{-3}T + 1.128\text{x}10^{-6}T^{2} + 3.965\text{x}10^{2}T^{-1} - 6.006$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf° = -77.599 - 0.093\text{x}10^{-3}T - 1.198\text{x}10^{-6}T^{2} - 79.400T^{-1}$
$\Delta Gf° = -77.599 + 0.093\text{x}10^{-3}T\ln T + 1.198\text{x}10^{-6}T^{2} - 39.700T^{-1} + 1.766\text{x}10^{-3}T$
1136-2125 K: $\Delta Hf° = -80.095 + 1.076\text{x}10^{-3}T - 1.067\text{x}10^{-6}T^{2} - 24.900T^{-1}$
$\Delta Gf° = -80.095 - 1.076\text{x}10^{-3}T\ln T + 1.067\text{x}10^{-6}T^{2} - 12.450T^{-1} + 12.315\text{x}10^{-3}T$
2125-2350 K: $\Delta Hf° = -81.998 - 2.100\text{x}10^{-3}T - 0.256\text{x}10^{-6}T^{2} - 46.500T^{-1}$
$\Delta Gf° = -81.998 + 2.100\text{x}10^{-3}T\ln T + 0.256\text{x}10^{-6}T^{2} - 23.250T^{-1} - 9.396\text{x}10^{-3}T$
2350-3000 K: $\Delta Hf° = -100.778 - 7.654\text{x}10^{-3}T + 1.128\text{x}10^{-6}T^{2} + 396.500T^{-1}$
$\Delta Gf° = -100.778 + 7.654\text{x}10^{-3}T\ln T - 1.128\text{x}10^{-6}T^{2} + 198.250T^{-1} - 41.304\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Other data from JANAF (127) who extrapolated above 2500 K.

ZrC$_{0.96}$(c)
Zirconium Carbide
[Formation: Zr(c,l) + 0.96C(c) = ZrC$_{0.96}$(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	9.015	7.930	7.930	0	-48.300	-47.493	34.813
300	9.060	7.986	7.930	.017	-48.298	-47.487	34.594
400	10.583	10.835	8.307	1.011	-48.178	-47.234	25.807
500	11.225	13.275	9.065	2.105	-48.055	-47.013	20.549
600	11.536	15.352	9.944	3.245	-47.969	-46.813	17.051
700	11.705	17.144	10.847	4.408	-47.926	-46.624	14.557
800	11.810	18.715	11.735	5.584	-47.926	-46.440	12.687
900	11.890	20.110	12.589	6.769	-47.963	-46.252	11.231
1000	11.964	21.367	13.405	7.962	-48.031	-46.059	10.066
1100	12.044	22.511	14.182	9.162	-48.128	-45.847	9.109
1136	12.077	22.899	14.452	9.596	-48.170	-45.772	8.806
1136	12.077	22.899	14.452	9.596	-49.121	-45.772	8.806
1200	12.135	23.563	14.920	10.371	-49.109	-45.593	8.304
1300	12.243	24.538	15.623	11.590	-49.105	-45.301	7.616
1400	12.371	25.450	16.293	12.820	-49.113	-45.008	7.026
1500	12.519	26.308	16.931	14.065	-49.133	-44.713	6.515
1600	12.690	27.122	17.544	15.325	-49.159	-44.418	6.067
1700	12.885	27.897	18.131	16.603	-49.190	-44.123	5.672
1800	13.103	28.639	18.693	17.903	-49.221	-43.822	5.321
1900	13.347	29.354	19.236	19.225	-49.250	-43.523	5.006
2000	13.615	30.046	19.760	20.573	-49.275	-43.221	4.723
2100	13.909	30.717	20.265	21.949	-49.292	-42.918	4.466
2125	13.989	30.882	20.389	22.298	-49.295	-42.843	4.406
2125	13.989	30.882	20.389	22.298	-54.295	-42.843	4.406
2200	14.228	31.371	20.755	23.355	-54.274	-42.440	4.216
2300	14.573	32.011	21.231	24.795	-54.220	-41.900	3.981
2400	14.944	32.639	21.693	26.271	-54.134	-41.366	3.767
2500	15.341	33.257	22.143	27.785	-54.012	-40.838	3.570
2600	15.764	33.867	22.582	29.340	-53.854	-40.314	3.389
2700	16.213	34.470	23.011	30.939	-53.655	-39.795	3.221
2800	16.689	35.068	23.431	32.584	-53.413	-39.286	3.066
2900	17.191	35.663	23.843	34.277	-53.126	-38.787	2.923
3000	17.719	36.254	24.246	36.023	-52.790	-38.297	2.790

Phase changes: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.
2125 K, melting point of Zr; ΔH° = 5.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.749 + 0.676\times10^{-3}T - 2.605\times10^{5}T^{-2}$
$H°-H°_{298} = 11.749\times10^{-3}T + 0.338\times10^{-6}T^{2} + 2.605\times10^{2}T^{-1} - 4.407$
2000-3200 K: $Cp° = 5.450 + 4.002\times10^{-3}T$
$H°-H°_{298} = 5.450\times10^{-3}T + 2.001\times10^{-6}T^{2} + 1.669$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf° = -49.099 + 2.379\times10^{-3}T - 1.339\times10^{-6}T^{2} + 62.192T^{-1}$
$\Delta Gf° = -49.099 - 2.379\times10^{-3}T\ln T + 1.339\times10^{-6}T^{2} + 31.096T^{-1} + 18.190\times10^{-3}T$
1136-2000 K: $\Delta Hf° = -51.595 + 3.548\times10^{-3}T - 1.208\times10^{-6}T^{2} + 116.692T^{-1}$
$\Delta Gf° = -51.595 - 3.548\times10^{-3}T\ln T + 1.208\times10^{-6}T^{2} + 58.346T^{-1} + 28.739\times10^{-3}T$
2000-2125 K: $\Delta Hf° = -43.606 - 4.789\times10^{-3}T + 1.061\times10^{-6}T^{2} - 669.600T^{-1}$
$\Delta Gf° = -43.606 + 4.789\times10^{-3}T\ln T - 1.061\times10^{-6}T^{2} - 334.800T^{-1} - 33.987\times10^{-3}T$
2125-3000 K: $\Delta Hf° = -45.509 - 7.965\times10^{-3}T + 1.872\times10^{-6}T^{2} - 691.200T^{-1}$
$\Delta Gf° = -45.509 + 7.965\times10^{-3}T\ln T - 1.872\times10^{-6}T^{2} - 345.600T^{-1} - 55.698\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Baker (16). Other data from Storms (476).

ZrH(g)
Zirconium Hydride (ideal gas)
[Formation: $Zr(c) + 0.5H_2(g) = ZrH(g)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.096	51.638	51.638	0	123.400	115.435	-84.615
300	7.099	51.682	51.639	.013	123.396	115.386	-84.057
400	7.348	53.756	51.918	.735	123.131	112.756	-61.606
500	7.632	55.426	52.458	1.484	122.863	110.194	-48.165
600	7.891	56.841	53.074	2.260	122.597	107.683	-39.223
700	8.108	58.075	53.702	3.061	122.334	105.219	-32.850
800	8.284	59.169	54.319	3.880	122.065	102.791	-28.081
900	8.427	60.153	54.913	4.716	121.791	100.399	-24.380
1000	8.543	61.048	55.483	5.565	121.507	98.037	-21.426
1100	8.639	61.866	56.026	6.424	121.209	95.705	-19.015
1136	8.668	62.145	56.216	6.736	121.097	94.872	-18.252
1136	8.668	62.145	56.216	6.736	120.146	94.872	-18.252
1200	8.719	62.622	56.545	7.292	120.035	93.451	-17.020
1300	8.787	63.322	57.039	8.168	119.852	91.244	-15.339
1400	8.845	63.976	57.512	9.049	119.653	89.050	-13.901
1500	8.896	64.588	57.964	9.936	119.437	86.871	-12.657
1600	8.942	65.163	58.396	10.828	119.205	84.708	-11.570
1700	8.982	65.707	58.810	11.725	118.958	82.559	-10.614
1800	9.019	66.221	59.207	12.625	118.693	80.425	-9.765
1900	9.053	66.710	59.590	13.528	118.410	78.305	-9.007
2000	9.084	67.175	59.958	14.435	118.110	76.203	-8.327

*Data estimated.

Phase change: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.431 + 1.032\times10^{-3}T - 0.571\times10^{5}T^{-2}$

$H°- H°_{298} = 7.431\times10^{-3}T + 0.516\times10^{-6}T^{2} + 0.571\times10^{2}T^{-1} - 2.453$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf° = 123.881 - 1.790\times10^{-3}T - 0.636\times10^{-6}T^{2} + 32.450T^{-1}$

$\Delta Gf° = 123.881 + 1.790\times10^{-3}T\ln T + 0.636\times10^{-6}T^{2} + 16.225T^{-1} - 38.900\times10^{-3}T$

1136-2000 K: $\Delta Hf° = 121.385 - 0.621\times10^{-3}T - 0.505\times10^{-6}T^{2} + 86.950T^{-1}$

$\Delta Gf° = 121.385 + 0.621\times10^{-3}T\ln T + 0.505\times10^{-6}T^{2} + 43.475T^{-1} - 28.350\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

ZrN(c)
Zirconium Nitride
[Formation: Zr(c) + $0.5N_2(g)$ = ZrN(c)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.650	9.290	9.290	0	-87.200	-80.368	58.910
300	9.681	9.350	9.290	.018	-87.200	-80.325	58.516
400	10.788	12.304	9.684	1.048	-87.158	-78.038	42.637
500	11.374	14.780	10.464	2.158	-87.066	-75.768	33.118
600	11.748	16.889	11.362	3.316	-86.957	-73.518	26.779
700	12.022	18.722	12.286	4.505	-86.844	-71.288	22.257
800	12.242	20.342	13.194	5.718	-86.738	-69.074	18.870
900	12.431	21.795	14.071	6.952	-86.637	-66.871	16.238
1000	12.601	23.114	14.910	8.204	-86.548	-64.680	14.136
1100	12.759	24.322	15.711	9.472	-86.468	-62.496	12.417
1136	12.812	24.734	15.991	9.932	-86.442	-61.712	11.872
1136	12.812	24.734	15.991	9.932	-87.393	-61.712	11.872
1200	12.907	25.439	16.476	10.755	-87.258	-60.269	10.976
1300	13.050	26.477	17.205	12.053	-87.052	-58.028	9.755
1400	13.188	27.450	17.904	13.365	-86.853	-55.803	8.711
1500	13.323	28.364	18.570	14.691	-86.660	-53.591	7.808
1600	13.455	29.228	19.209	16.030	-86.475	-51.393	7.020
1700	13.586	30.048	19.823	17.382	-86.295	-49.207	6.326
1800	13.715	30.828	20.413	18.747	-86.121	-47.030	5.710
1900	13.843	31.573	20.981	20.125	-85.952	-44.864	5.160
2000	13.970	32.286	21.528	21.515	-85.790	-42.705	4.667

Phase change: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 11.594 + 1.214\text{x}10^{-3}T - 2.067\text{x}10^{5}T^{-2}$

$H°- H°_{298} = 11.594\text{x}10^{-3}T + 0.607\text{x}10^{-6}T^{2} + 2.067\text{x}10^{2}T^{-1} - 4.204$

Formation equations (kcal/mol):

298.15-1136 K: $ΔHf° = -88.439 + 2.342\text{x}10^{-3}T - 0.629\text{x}10^{-6}T^{2} + 177.750T^{-1}$

$ΔGf° = -88.439 - 2.342\text{x}10^{-3}T\ln T + 0.629\text{x}10^{-6}T^{2} + 88.875T^{-1} + 39.229\text{x}10^{-3}T$

1136-2000 K: $ΔHf° = -90.935 + 3.512\text{x}10^{-3}T - 0.499\text{x}10^{-6}T^{2} + 232.250T^{-1}$

$ΔGf° = -90.935 - 3.512\text{x}10^{-3}T\ln T + 0.499\text{x}10^{-6}T^{2} + 116.125T^{-1} + 49.778\text{x}10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Low-temperature heat capacities and entropy at 298 K from Todd (493). High-temperature data based on Coughlin (101).

ZrN(g)
Zirconium Nitride (ideal gas)
[Formation: Zr(c) + $0.5N_2(g)$ = ZrN(g)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.567	55.780	55.780	0	134.000	126.971	-93.071
300	7.575	55.827	55.780	.014	133.997	126.928	-92.466
400	7.965	58.062	56.082	.792	133.786	124.603	-68.079
500	8.243	59.871	56.665	1.603	133.578	122.331	-53.470
600	8.434	61.392	57.329	2.438	133.365	120.102	-43.746
700	8.567	62.703	58.006	3.288	133.138	117.909	-36.812
800	8.664	63.853	58.666	4.150	132.894	115.749	-31.621
900	8.736	64.878	59.300	5.020	132.631	113.623	-27.591
1000	8.791	65.802	59.905	5.897	132.345	111.525	-24.373
1100	8.835	66.642	60.480	6.778	132.038	109.458	-21.747
1136	8.848	66.927	60.680	7.096	131.922	108.720	-20.916
1136	8.848	66.927	60.680	7.096	130.971	108.720	-20.916
1200	8.871	67.412	61.026	7.663	130.850	107.471	-19.573
1300	8.901	68.123	61.545	8.552	130.646	105.531	-17.741
1400	8.926	68.784	62.039	9.443	130.425	103.607	-16.174
1500	8.948	69.400	62.509	10.337	130.186	101.701	-14.818
1600	8.968	69.978	62.957	11.233	129.928	99.810	-13.633
1700	8.985	70.523	63.388	12.130	129.653	97.934	-12.590
1800	9.001	71.037	63.798	13.030	129.362	96.076	-11.665
1900	9.016	71.524	64.192	13.931	129.053	94.235	-10.839
2000	9.029	71.986	64.570	14.833	128.728	92.413	-10.098

*Data estimated.

Phase change: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.439 + 0.382\times10^{-3}T - 0.876\times10^{5}T^{-2}$

$H°-H°_{298} = 8.439\times10^{-3}T + 0.191\times10^{-6}T^{2} + 0.876\times10^{2}T^{-1} - 2.827$

Formation equations (kcal/mol):

298.15-1136 K: $ΔHf° = 134.138 - 0.813\times10^{-3}T - 1.045\times10^{-6}T^{2} + 58.650T^{-1}$

$ΔGf° = 134.138 + 0.813\times10^{-3}T\ln T + 1.045\times10^{-6}T^{2} + 29.325T^{-1} - 29.310\times10^{-3}T$

1136-2000 K: $ΔHf° = 131.642 + 0.357\times10^{-3}T - 0.915\times10^{-6}T^{2} + 113.150T^{-1}$

$ΔGf° = 131.642 - 0.357\times10^{-3}T\ln T + 0.915\times10^{-6}T^{2} + 56.575T^{-1} - 18.761\times10^{-3}T$

Source: Data are those estimated by JANAF (127).

$Zr(SO_4)_2(c)$
Zirconium Sulfate
[Reaction: $Zr(c) + S_2(g) + 4O_2(g) = Zr(SO_4)_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	37.828	31.800	31.800	0	-566.910	-498.918	365.712
300	38.183	32.035	31.802	.070	-566.917	-498.495	363.149
400	49.836	44.904	33.477	4.571	-566.694	-475.696	259.905
500	53.978	56.550	36.954	9.798	-565.885	-453.031	198.017
600	55.165	66.525	41.073	15.271	-564.972	-430.546	156.824
700	54.955	75.025	45.332	20.785	-564.144	-408.209	127.447
800	54.001	82.308	49.512	26.237	-563.490	-385.984	105.445
900	52.615	88.591	53.512	31.571	-563.046	-363.823	88.347
1000	50.961	94.051	57.299	36.752	-562.835	-341.701	74.678
1050	50.063	96.516	59.109	39.277	-562.825	-330.644	68.820

*Entropy at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1050 K: $Cp° = 77.138 - 23.302\times10^{-3}T - 28.768\times10^{5}T^{-2}$
$H°- H°_{298} = 77.138\times10^{-3}T - 11.651\times10^{-6}T^{2} + 28.768\times10^{2}T^{-1} - 31.612$

Reaction equations (kcal/mol):

298.15-1050 K: $\Delta Hr° = -584.388 + 33.882\times10^{-3}T - 14.925\times10^{-6}T^{2} + 2594.800T^{-1}$
$\Delta Gr° = -584.388 - 33.882\times10^{-3}T\ln T + 14.925\times10^{-6}T^{2} + 1297.400T^{-1} + 460.669\times10^{-3}T$

Source: Data from DeKock (113) who estimated entropy at 298 K.

$ZrSiO_4(c)$
Zirconium Silicate
[Formation: $Zr(c) + Si(c,l) + 2O_2(g) = ZrSiO_4(c)$]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	23.560	20.100	20.100	0	-486.000	-458.651	336.196
300	23.679	20.246	20.100	.044	-486.002	-458.480	333.998
400	28.019	27.728	21.091	2.655	-485.958	-449.307	245.487
500	30.314	34.250	23.086	5.582	-485.706	-440.168	192.395
600	31.775	39.914	25.429	8.691	-485.371	-431.093	157.023
700	32.823	44.895	27.862	11.923	-484.999	-422.076	131.776
800	33.635	49.333	30.274	15.247	-484.611	-413.115	112.856
900	34.294	53.333	32.616	18.645	-484.215	-404.199	98.152
1000	34.846	56.976	34.873	22.103	-483.814	-395.322	86.396
1100	35.315	60.320	37.037	25.611	-483.415	-386.500	76.789
1136	35.459	61.460	37.793	26.885	-483.272	-383.330	73.746
1136	35.459	61.460	37.793	26.885	-484.223	-383.330	73.746
1200	35.716	63.410	39.108	29.163	-483.876	-377.654	68.779
1300	36.059	66.283	41.088	32.753	-483.335	-368.826	62.004
1400	36.350	68.966	42.985	36.373	-482.802	-360.033	56.203
1500	36.594	71.483	44.802	40.021	-482.276	-351.295	51.183
1600	36.793	73.851	46.544	43.691	-481.763	-342.581	46.794
1687	36.930	75.803	48.004	46.898	-481.329	-335.004	43.399
1687	36.930	75.803	48.004	46.898	-493.411	-335.004	43.399
1700	36.950	76.087	48.218	47.378	-493.338	-333.779	42.910
1800	37.066	78.202	49.825	51.079	-492.790	-324.405	39.388
1900	37.142	80.208	51.371	54.790	-492.260	-315.066	36.240
2000	37.179	82.114	52.861	58.507	-491.750	-305.758	33.411

Phase changes: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 32.422 + 3.058\times10^{-3}T - 8.688\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 32.422\times10^{-3}T + 1.529\times10^{-6}T^2 + 8.688\times10^{2}T^{-1} - 12.717$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf^\circ = -489.977 + 6.290\times10^{-3}T - 0.770\times10^{-6}T^2 + 647.000T^{-1}$
$\Delta Gf^\circ = -489.977 - 6.290\times10^{-3}T\ln T + 0.770\times10^{-6}T^2 + 323.500T^{-1} + 137.038\times10^{-3}T$
1136-1687 K: $\Delta Hf^\circ = -492.473 + 7.459\times10^{-3}T - 0.639\times10^{-6}T^2 + 701.500T^{-1}$
$\Delta Gf^\circ = -492.473 - 7.459\times10^{-3}T\ln T + 0.639\times10^{-6}T^2 + 350.750T^{-1} + 147.587\times10^{-3}T$
1687-2000 K: $\Delta Hf^\circ = -504.902 + 7.038\times10^{-3}T - 0.288\times10^{-6}T^2 + 800.000T^{-1}$
$\Delta Gf^\circ = -504.902 - 7.038\times10^{-3}T\ln T + 0.288\times10^{-6}T^2 + 400.000T^{-1} + 152.401\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (515). Low-temperature heat capacities and entropy at 298 K from Kelley (240). High-temperature data based on Coughlin (101).

$ZrTe_2(c)$
Zirconium Ditelluride
[Reaction: $Zr(c) + Te_2(g) = ZrTe_2(c)$]

T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHr°	ΔGr°	
298.15	17.713	29.694	29.694	0	-108.630	-96.258	70.558
300	17.727	29.804	29.694	.033	-108.624	-96.182	70.067
400	18.212	34.974	30.396	1.831	-108.345	-92.077	50.308
500	18.585	39.080	31.736	3.672	-108.067	-88.040	38.482
600	18.920	42.498	33.253	5.547	-107.797	-84.057	30.617
700	19.240	45.437	34.787	7.455	-107.531	-80.122	25.015
800	19.560	48.028	36.284	9.395	-107.272	-76.228	20.824
900	19.883	50.351	37.721	11.367	-107.015	-72.364	17.572
1000	20.213	52.462	39.090	13.372	-106.763	-68.527	14.976
1100	20.550	54.405	40.397	15.409	-106.513	-64.713	12.857
1136	20.674	55.069	40.851	16.151	-106.423	-63.347	12.187
1136	20.674	55.069	40.851	16.151	-107.374	-63.347	12.187
1200	20.894	56.207	41.639	17.482	-107.123	-60.869	11.086
1300	21.248	57.894	42.826	19.589	-106.728	-57.033	9.588
1400	21.613	59.481	43.958	21.732	-106.328	-53.225	8.309
1500	21.989	60.985	45.044	23.912	-105.912	-49.448	7.204

Phase change: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 17.114 + 3.160 \times 10^{-3}T - 0.305 \times 10^{5}T^{-2}$
$H° - H°_{298} = 17.114 \times 10^{-3}T + 1.580 \times 10^{-6}T^{2} + 0.305 \times 10^{2}T^{-1} - 5.345$

Reaction equations (kcal/mol):

298.15-1136 K: $\Delta Hr° = -109.297 + 2.522 \times 10^{-3}T + 0.045 \times 10^{-6}T^{2} - 26.600T^{-1}$
$\Delta Gr° = -109.297 - 2.522 \times 10^{-3}T\ln T - 0.045 \times 10^{-6}T^{2} - 13.300T^{-1} + 58.265 \times 10^{-3}T$
1136-1500 K: $\Delta Hr° = -111.793 + 3.691 \times 10^{-3}T + 0.176 \times 10^{-6}T^{2} + 27.900T^{-1}$
$\Delta Gr° = -111.793 - 3.691 \times 10^{-3}T\ln T - 0.176 \times 10^{-6}T^{2} + 13.950T^{-1} + 68.814 \times 10^{-3}T$

Source: Data from Johnson (220).

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[3] A title in parentheses is a translation from the language in which the reference was published.

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