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**THERMOPHYSICAL PROPERTIES OF
THORIUM AND URANIUM SYSTEMS
FOR USE IN REACTOR SAFETY ANALYSIS**

by

**Joanne K. Fink, Martin G. Chasanov,
and Leonard Leibowitz**

U of C-AUA-USERDA

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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Chemical Engineering Division

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INTRODUCTION

The data presented in this compilation are intended to serve as a preliminary set of thermophysical property values for use by workers engaged in reactor safety analyses of the Th-²³³U reactor concept. The data were obtained from currently available reviews and data collections. The primary sources of information are given in Refs. 1-4. In some cases, when data were not available and we thought that the results were justifiable, we have provided "best" estimates of the values for these properties. In such cases, the estimation techniques are discussed. Work is in progress to provide error estimates for cases in which that information is now lacking. These estimates will be included in future revisions of this report.

It should be clear from this compilation that much experimental work needs to be done to provide a firm data base for reactor calculations involving thorium-uranium systems. We plan to update this initial effort by continuing our search of the literature for new data and by applying appropriate theoretical methods to the estimation of additional data for these systems. In the interim, we believe that the material presented here will enable designers and analysts to make computations that should provide reasonable results.

In this compilation, we have included the thermophysical properties of various thorium, uranium, and thorium-uranium systems. Following each recommended value of a property there is a discussion which includes the methods of estimation, equations used, sources of the calculations, and the experimental sources.

First, the thermophysical properties of Th, U, and Th_{0.9}U_{0.1} are discussed; then the properties of ThO₂, UO₂, and (Th_{0.9}U_{0.1})O₂; and finally the properties of the mono and dicarbides of Th, U, and Th_{0.9}U_{0.1}. The ratio of 0.9 Th to 0.1 U was chosen for the mixed thorium-uranium system because that was the best estimate of an appropriate ratio at the time this report was compiled. Since it is realized that other ratios are likely to be considered, the method used to obtain values for the mixture has been explained in the discussion of each property. Thus, the reader may calculate the value of a property for a different ratio by using the appropriate method for the cases in which the value has been calculated and not obtained by experimental measurement.

The properties of (Pu_{0.2}U_{0.8})O₂ and of (Pu_{0.2}U_{0.8})C have also been included, in appropriate order, since these have been considered as reactor fuels in many reactor safety analyses; thus, comparisons of their properties with those of (Th_{0.9}U_{0.1})O₂ and (Th_{0.9}U_{0.1})C may be desired. This comparison by the analyst may serve to give him an insight into the effects he can expect in his calculations and computer codes in changing from the Pu_{0.2}U_{0.8} system to the Th_{0.9}U_{0.1} system.

To aid in the comparison of properties of uranium systems and thorium systems, five graphs have been included in the appendix. These graphs include comparisons of enthalpy, heat capacity and vapor pressure of ThO_2 and UO_2 . Plots of the vapor pressure of Th and U as a function of temperature are also included.

For the user's convenience in comparison of properties and for quick reference, three tables summarizing the values of thermophysical properties discussed in the compilation are included below. The order of the properties and materials in the tables follows the order in the text. Table 1a gives the thermophysical properties of the metals: Th, $\text{Th}_{0.9}\text{U}_{0.1}$, and U. The properties of the oxides ThO_2 , $(\text{Th}_{0.9}\text{U}_{0.1})\text{O}_2$, UO_2 , and $(\text{Pu}_{0.2}\text{U}_{0.8})\text{O}_2$ are given in Table 1b. The last table, Table 1c, contains the properties of monocarbides and dicarbides: ThC , $(\text{Th}_{0.9}\text{U}_{0.1})\text{C}$, UC , $(\text{Pu}_{0.2}\text{U}_{0.8})\text{C}$, ThC_2 , $(\text{Th}_{0.9}\text{U}_{0.1})\text{C}_2$, and UC_2 . The values of properties that are in roman type are values obtained by experimental measurements. Those values that are in italics have been obtained by calculation or an estimation technique which is explained in the appropriate section of the text. The symbols used in Tables 1a, b, and c, and throughout the body of the report, are defined as follows:

T = temperature

P = pressure

$H_{(\text{MP})}$ = enthalpy at the melting point

$H_{(298)}$ = enthalpy at 298 K

ΔH_m = heat of fusion

$\Delta H_{V(298)}$ = heat of vaporization at 298 K

$\Delta H_{V(\text{BP})}$ = heat of vaporization at the boiling point

$H_{(\text{BP})}$ = enthalpy at the boiling point

$C_{P(298)}$ = molar heat capacity at 298 K

$C_{P(\text{MP})}^{(s)}$ = molar heat capacity of the solid at the melting point

$C_{P(\text{MP})}^{(l)}$ = molar heat capacity of the liquid at the melting point

$C_{P(\text{BP})}^{(l)}$ = molar heat capacity of the liquid at the boiling point

$K_{(298)}^{(s)}$ = thermal conductivity at 298 K

$K_{(MP)}^{(s)}$ = thermal conductivity of the solid at the melting point

$K_{(MP)}^{(l)}$ = thermal conductivity of the liquid at the melting point

$K_{(BP)}^{(l)}$ = thermal conductivity of the liquid at the boiling point

ϵ_T = normal total emissivity

$\epsilon(0.65 \mu\text{m})$ = normal spectral emissivity at $0.65 \mu\text{m}$

$\rho_{(298)}^{(s)}$ = density of the solid at 298 K

$\rho_{(MP)}^{(s)}$ = density of the solid at the melting point

$\left(-\frac{\Delta\rho}{\rho}\right)_{MP}$ = fractional change in density on melting

$\rho_{(BP)}^{(l)}$ = density of the liquid at the boiling point

$\bar{\alpha}^{(s)}$ = average volumetric expansion coefficient of the solid

$\bar{\alpha}_{(MP)}^{(l)}$ = average volumetric expansion coefficient of the liquid at the melting point

κ_s = adiabatic compressibility

κ_T = isothermal compressibility

$\nu_{(MP)}$ = viscosity of the liquid at the melting point

σ = surface tension

Table 1a. Thermophysical Properties of Metals and Alloys

Property	Th	Th _{0.9} U _{0.1}	U
Melting Point (K)	2023±15	1815	1408
Boiling Point (K)	4975	4892	4427
Critical Temp. (K)	-	-	-
Critical Pressure (Pa)	-	-	-
H _(MP) - H ₍₂₉₈₎ (kJ/mol)	62.22	60.92	49.20
ΔH _m (kJ/mol)	13.8±1.2	10.9	9.1
H _(BP) - H ₍₂₉₈₎ (kJ/mol)	211.7	210.5	205.0
ΔH _V (kJ/mol) (298)	597.1±13	536	531 ⁺⁸ ₋₄
ΔH _V (kJ/mol) (BP)	-	-	-
C _P (298) (J/K·mol)	27.32±0.29	27.36	27.66
C _P (s) (J/K·mol) (MP)	39.87	39.7	38.28
C _P (l) (J/K·mol) (MP)	46	46.4	48.66
C _P (l) (J/K·mol) (BP)	-	-	-
K ₍₂₉₈₎ (W/m·K)	49.1	46	27.6
K _(MP) (s) (W/m·K)	-	-	-
K _(MP) (l) (W/m·K)	-	-	-
K _(BP) (l) (W/m·K)	-	-	-
E _T	-	-	-
F (0.65 μm)	-	-	-
ρ ₍₂₉₈₎ (s) (kg/m ³)	1.17x10 ⁴	1.24x10 ⁴	1.90x10 ⁴
ρ _(MP) (s) (kg/m ³)	1.10x10 ⁴	1.16x10 ⁴	1.74x10 ⁴
$\left(-\frac{\Delta\rho}{\rho}\right)_{MP}$	-	-	-
ρ _(BP) (l) (kg/m ³)	-	-	-
α _(298-MP) (s) (K ⁻¹)	3.5x10 ⁻⁵	-	6x10 ⁻⁵ (α) 5x10 ⁻⁵ (β) 7x10 ⁻⁵ (γ)
α _(MP) (l) (K ⁻¹)	-	-	-
κ _S (Pa ⁻¹)	-	-	-
κ _T (Pa ⁻¹)	-	-	-
ν _(MP) (Pa·s)	-	-	-
σ (N/m)	-	-	-
T of Phase Transitions (K)	1633±10(α+β)	-	940.9±1(α+β) 1048.0±1.6(β+γ)

Table 1b. Thermophysical Properties of Oxides

Property	ThO ₂	(Th _{0.9} U _{0.1})O ₂	UO ₂	(U _{0.8} Pu _{0.2})O ₂
Melting Point (K)	3643±30	3500	3138±15	3063(ℓ) 3023(s)
Boiling Point (K)	4320	4250	3760±200	3520
Critical Temp., (K)	-	-	-	-
Critical Pressure (Pa)	-	-	-	-
H _(MP) - H ₍₂₉₈₎ (kJ/mol)	290.4	265.6	310.0	282.5
ΔH _m (kJ/mol)	90.8	87.4	74.9±1.2	74.9±1.2
H _(BP) - H ₍₂₉₈₎ (kJ/mol)	484.1	471.1	469.4	425.5
ΔH _V (298) (kJ/mol)	664.0±10.5	602	598	619
ΔH _V (BP) (kJ/mol)	-	-	454±53	536±54
C _P (298) (J/K·mol)	61.73	64.27	63.6	69.6
C _P ^(s) (MP) (J/K·mol)	103.2	95	208.4	173.3
C _P ^(ℓ) (MP) (J/K·mol)	136.0	136.0	136.0	136.0
C _P ^(ℓ) (BP) (J/K·mol)	136.0	136.0	136.0	136.0
K ₍₂₉₈₎ (W/m·K)	13.2	11.1	8.4	6.3
K _(MP) ^(s) (W/m·K)	-	-	-	-
K _(MP) ^(ℓ) (W/m·K)	-	-	-	-
K _(BP) ^(ℓ) (W/m·K)	-	-	-	-
ε _T	-	-	-	-
ε(0.65 μm)	-	-	0.87±0.1	0.87±0.1
ρ ₍₂₉₈₎ ^(s) (kg/m ³)	(1.0013±0.0001)×10 ⁴	1.009×10 ⁴	1.097×10 ⁴	1.108×10 ⁴
ρ _(MP) ^(s) (kg/m ³)	8.8×10 ³	8.8×10 ³	9.1×10 ³	9.88×10 ³
$\left(-\frac{\Delta\rho}{\rho}\right)_{MP}$	0.11	0.11	0.11	0.11
ρ _(BP) ^(ℓ) (kg/m ³)	-	-	-	-
$\bar{\alpha}_{(298-MP)}^{(s)}$ (K ⁻¹)	3.5×10 ⁻⁵	3.5×10 ⁻⁵	4.5×10 ⁻⁵	4.5×10 ⁻⁵
$\bar{\alpha}_{(MP)}^{(ℓ)}$ (K ⁻¹)	9×10 ⁻⁵	9×10 ⁻⁵	9×10 ⁻⁵	9×10 ⁻⁵
κ _(s) (Pa ⁻¹)	-	-	-	-
κ _T (Pa ⁻¹)	-	-	-	-
ν _(MP) (Pa·s)	(4.30±0.1)×10 ⁻³	(4.30±0.1)×10 ⁻³	(4.30±0.1)×10 ⁻³	(4.30±0.1)×10 ⁻³
σ (N/m)	-	-	0.45±0.04	0.45±0.04
T of Phase Transitions (K)	-	-	-	-

Table 1c. Thermophysical Properties of Carbides

Property	ThC	(Th _{0.9} U _{0.1})C	UC	(U _{0.8} Pu _{0.2})C
Melting Point (K)	2773±35	2775	2780±25	2780(ℓ) 2548(s)
Boiling Point (K)	-	-	4800	4560
Critical Temp. (K)	-	-	9750	9653
Critical Pressure (Pa)	-	-	-	-
H _(MP) - H ₍₂₉₈₎ (kJ/mol)	155.2	156.9	171.33	152.3
ΔH _m (kJ/mol)	46	46	46	45.6
H _(BP) - H ₍₂₉₈₎ (kJ/mol)	-	-	372	351.5
ΔH _V ₍₂₉₈₎ (kJ/mol)	-	-	536	536
ΔH _V _(BP) (kJ/mol)	-	-	-	-
C _P ₍₂₉₈₎ (J/K·mol)	45.2±0.4	46.0	50.2	46.4
C _P ^(s) _(MP) (J/K·mol)	53.0	74.9	87.4	106.8
C _P ^(ℓ) _(MP) (J/K·mol)	71	71	71	71
C _P ^(s) _(BP) (J/K·mol)	-	-	87.4	84.9
K ₍₂₉₈₎ (W/m·K)	12	12	22	17
K _(MP) ^(s) (W/m·K)	-	-	24	23
K _(MP) ^(ℓ) (W/m·K)	-	-	20	20
K _(BP) ^(ℓ) (W/m·K)	-	-	-	-
ε _T	-	-	0.42±0.03	-
ε(0.65 μm)	-	-	0.539-2x10 ⁻⁵ T	-
ρ ₍₂₉₈₎ ^(s) (kg/m ³)	1.06x10 ⁴	1.09x10 ⁴	1.36x10 ⁴	1.35x10 ⁴
ρ _(MP) ^(s) (kg/m ³)	1.02x10 ⁴	1.04x10 ⁴	1.23x10 ⁴	1.23x10 ⁴
$\left(\frac{\Delta \rho}{\rho}\right)_{MP}$	-	-	-	-
ρ _(BP) ^(ℓ) (kg/m ³)	-	-	8.5x10 ³	8.6x10 ³
α _(298-MP) ^(s) (K ⁻¹)	1.7x10 ⁻⁵	2.0x10 ⁻⁵	3.9x10 ⁻⁵	3.4x10 ⁻⁵
α _(MP) ^(ℓ) (K ⁻¹)	-	-	8x10 ⁻⁵	6.8x10 ⁻⁵
κ _s (Pa ⁻¹)	-	-	-	-
κ _T (Pa ⁻¹)	-	-	7.1x10 ⁻¹²	-
ν _(MP) (Pa·s)	-	-	8x10 ⁻³	7x10 ⁻³
σ (N/m)	-	-	-	-
T of Phase Transitions (K)	-	-	-	-

Table 1c. (Cont'd.)

Property	ThC ₂	(Th _{0.9} U _{0.1})C ₂	UC ₂
Melting Point (K)	2913±30	2900	2780
Boiling Point (K)	5400	-	-
Critical Temp. (K)	-	-	-
Critical Pressure (Pa)	-	-	-
H _(MP) - H ₍₂₉₈₎ (kJ/mol)	218	222	256.0
ΔH _m (kJ/mol)	71	67	67
H _(BP) - H ₍₂₉₈₎ (kJ/mol)	-	-	-
ΔH _{V(298)} (kJ/mol)	690	-	-
ΔH _{V(BP)} (kJ/mol)	-	-	-
C _{P(298)} (J/K·mol)	56.69±0.59	57.3	60.7
C _{P(MP)} ^(s) (J/K·mol)	83.6	87.9	123.0
C _{P(MP)} ^(l) (J/K·mol)	-	-	-
C _{P(BP)} ^(l) (J/K·mol)	-	-	-
K ₍₂₉₈₎ (W/m·K)	-	18.8	-
K _(MP) ^(s) (W/m·K)	-	-	-
K _(MP) ^(l) (W/m·K)	-	-	-
K _(BP) ^(l) (W/m·K)	-	-	-
ε _T	-	-	-
ε (0.65 μm)	-	-	-
ρ ₍₂₉₈₎ ^(s) (kg/m ³)	9.6x10 ³	9.8x10 ³	1.17x10 ⁴
ρ _(MP) ^(s) (kg/m ³)	9.0x10 ³	9.1x10 ³	1.06x10 ⁴
$\left(-\frac{\Delta\rho}{\rho}\right)_{MP}$	-	-	-
ρ _(BP) ^(l) (kg/m ³)	-	-	-
α _(298-MP) ^(s) (K ⁻¹)	7.8x10 ⁻⁵	2.7x10 ⁻⁵	4.0x10 ⁻⁵
α _(MP) ^(l) (K ⁻¹)	-	-	-
κ _s (Pa ⁻¹)	-	-	-
κ _T (Pa ⁻¹)	-	-	-
ν _(MP) (Pa·s)	-	-	-
σ (N/m)	-	-	-
T of Phase Transitions (K)	1427(α→β) 1490(β→γ)	-	-

THORIUM (Th)

Melting Point: 2023 $\pm$ 15 K

This is a weighted average from five experiments.¹ The experimental values are tabulated below.

Table 2. Measurements of the Melting Point of Thorium

Melting Point, K	Experimenter	Ref.
2020	Ackermann and Rauh (1972)	5
2027	Benz, Hoffman, and Rupert (1967)	6
2028	Chiotti and Gill (1961)	7
2033	Eash and Carlson (1960)	8
2028	Korbitz (1964)	9

Boiling Point: 4975 K

This is the value recommended in Ref. 1.

Enthalpy, $H_{(MP)} - H_{(298)}$: 62.22 kJ/mol

This value¹ is based on experiments of Levinson¹⁰ from 1269 to 2100 K. His are the only experiments to temperatures above the melting point. Inconsistencies exist between the high temperature enthalpy data of various experimenters.

Heat of Fusion, ΔH_m : 13.8 $\pm$ 1.2 kJ/mol

This is an experimental value from experiments of Levinson.¹⁰

Enthalpy, $H_{(BP)} - H_{(298)}$: 211.7 kJ/mol

This value is from tabulated values of enthalpy given in Ref. 1. The enthalpy of Th has been measured only to 2100 K.¹⁰

Heat of Vaporization, $\Delta H_{v(298)}$: 597.1 $\pm$ 13 kJ/mol

This value was calculated by Ackermann and Rauh¹¹ from their vapor pressure measurements in the temperature range from 2020 to 2500 K. Their equation for the log of the pressure is

$$\log P(\text{atm}) = -(29770 \pm 218)/T + (6.024 \pm 0.098) \quad (1)$$

converted to SI units, it becomes

$$\log P(\text{Pa}) = -(29770 \pm 218)/T + (11.030 \pm 0.098) \quad (2)$$

These data were selected over other data because the authors gave a complete description of the role of oxygen contamination and because their data showed no variation in ΔH_V when calculated by either the second or the third law method.

Heat Capacity, $C_{P(298)}^{(s)}$: $27.32 \pm 0.29 \text{ J/K}\cdot\text{mol}$

This value, recommended in Ref. 1, is from calorimetric measurements by Griffel and Skochdapole.¹² Rand² gives the following equation, which we have converted to SI units, for calculating heat capacity of the α phase for the temperature range from 298 to 1633 K:

$$C_p(\alpha \text{ phase})(\text{J/K mol}) = 25.48 + 7.82 \times 10^{-3} T - 0.510 \times 10^{-5} T^2 \quad (3)$$

This equation gives the value $27.24 \text{ J/K}\cdot\text{mol}$ at 298 K.

Heat Capacity, $C_{P(MP)}^{(s)}$: $39.87 \text{ J/K}\cdot\text{mol}$

This value is based on drop calorimetric measurements by Levinson on β -phase thorium in the temperature range from 1667 to 1991 K.¹⁰ His are the only experiments in this temperature region. High-temperature heat capacity data in the α phase are not completely consistent.¹ Rand² gives the following equation, which we have converted to SI units, for calculating heat capacity in the β phase for the temperature range from 1633 to 2023 K:

$$C_p(\beta \text{ phase})(\text{J/K mol}) = 15.69 + 11.97 \times 10^{-3} T \quad (4)$$

This equation gives 30.90 J/K mol at 2023 K.

Heat Capacity, $C_{P(MP)}^{(l)}$: $46.0 \text{ J/K}\cdot\text{mol}$

This value, taken from Ref. 1, is based only on two measurements of liquid enthalpy by Levinson.¹⁰

Thermal Conductivity, $K_{(298)}$: $49.1 \text{ W/m}\cdot\text{K}$

This is the value recommended by Touloukian¹³ and is based on an evaluation of six sets of measurements by nine authors. Measurements range from 5.3 K^{13a} to 923 K^{13b}

Density, $\rho_{(298)}^{(s)}$: $1.17 \times 10^4 \text{ kg/m}^3$

This value, cited by Ferro,² is based on the identical density values measured by James and Straumanis¹⁴ and calculated by Wyckoff¹⁵ from lattice parameters.

Density, $\rho_{(MP)}^{(s)}$: $1.10 \times 10^4 \text{ kg/m}^3$

This value was calculated by us using the thermal expansion coefficients tabulated by Touloukian.¹³

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(298\text{-MP})}^{(s)}$: $3.5 \times 10^{-5} \text{ K}^{-1}$

This value was taken from the compilation by Touloukian.¹³ It is based on his analysis of 17 sets of data by seven authors. Measurements have been made to 1273 K.^{15a}

Phase Transition, $\alpha \rightarrow \beta$: $1633 \pm 10 \text{ K}$

Experimental values¹⁶⁻²¹ for the α -to- β phase transition range from 1603 to 1678 K. The differences are believed due to impurities in the samples. The selected value¹ is based on experimental data of Chiotti and Gill¹⁷ and experimental data of Takeuchi *et al.*,²⁰ who both extrapolated the transition temperature to zero carbon content, and from experiments of McMasters and Larsen.¹⁸

THORIUM-URANIUM (Th_{0.9}U_{0.1})Melting Point: 1815 K

This value was taken from the thorium-uranium phase diagram.² The solidus-liquidus curve is due to Ackermann and Rauh.⁵

Boiling Point: 4892 K

The boiling point of the mixture was calculated by us. The value given is the temperature at which the total pressure of the mixture equals 1 atm. The total pressure was determined from the partial pressures by means of the equation

$$P = \sum_i P_i X_i \quad (5)$$

where

X_i = the mole fraction of the i^{th} component

P_i = the pressure of the i^{th} component

The maximum temperature at which the vapor pressures of U and of Th have been measured^{11,22} is 2500 K. Therefore, large extrapolations were needed to reach the boiling point. These were made by assuming that an equation of the form

$$\log P = A/T + B \quad (6)$$

was applicable over the entire temperature range of interest.

Enthalpy, $H_{(\text{MP})} - H_{(298)}$: 60.92 kJ/mol

The value 60.92 kJ/mol is a molar average* calculated by us. No experimental data exist.

Heat of Fusion, ΔH_m : 10.9 kJ/mol

A molar average was calculated by us since no experimental data exist.

Enthalpy, $H_{(\text{BP})} - H_{(298)}$: 210.5 kJ/mol

A molar average was calculated from our estimates for the pure components. No data exist for the alloy.

* In many cases, no data are available for mixtures. In these cases, a molar average value calculated from the pure components was used. This will be referred to simply as "molar average."

Heat of Vaporization, ΔH_V : 536 kJ/mol
(298)

The heat of vaporization was determined from the slope of a curve of $\log P$ vs. $1/T$, where P = pressure and T = temperature. Vapor pressure measurements^{11,22} have been made to 2500 K for U and Th.

Heat Capacity, C_P : 27.36 J/K·mol
(298)

Since there are no experimental measurements of heat capacity of Th_{0.9}U_{0.1}, a molar average is given for the heat capacity.

Heat Capacity, $C_P^{(s)}$: 39.7 J/K·mol
(MP)

This is a molar average. No experimental data exist.

Heat Capacity, $C_P^{(l)}$: 46.4 J/K·mol
(MP)

This is a molar average. No experimental data exist.

Thermal Conductivity, K : 46 W/m·K
(298)

This value was calculated assuming that the reciprocals of thermal conductivities of the components are additive.¹³ Thus, the equation used was

$$\frac{1}{K(\text{ThU})} = \frac{x}{K(\text{U})} + \frac{(1-x)}{K(\text{Th})} \quad (7)$$

where x = the mole fraction of U in ThU.

Density, ρ : 1.24 x 10⁴ kg/m³
(298)

This is a molar average. The density of Th_{0.9}U_{0.1} at 298 K has not been measured.

Density, ρ : 1.16 x 10⁴ kg/m³
(MP)

The density given is a molar average. No experimental data exist.

URANIUM (U)

Melting Point: 1408 ± 2 K

This value was recommended¹ on the basis of five experiments showing excellent agreement. The experimental values are given in Table 3.

Table 3. Measurements of Melting Point of Uranium

Melting Point, K	Temperature Scale	Experimenter	Ref.
1405.5 ± 0.8	IPTS-1948	Blumenthal	23
1406	IPTS-1948	Buzzard <i>et al.</i>	24
1405.5 ± 10	IPTS-1948	Udy and Boulger	25
1406 ± 2	IPTS-1948	Dahl and Cleaves	26
1408 ± 1	IPTS-1968	Ackermann and Rauh	5

Boiling Point: 4427 K

The boiling point of U was taken to be the temperature at which the vapor pressure equals 1 atm. Since vapor pressure measurements of U have been made only to 2500 K,²² extrapolations were performed by us assuming a constant heat of vaporization.

Enthalpy, $H_{(MP)} - H_{(298)}$: 49.20 kJ/mol

Enthalpy and heat capacity measurements at various temperatures have been made by several investigators, as shown in Table 4.

The change in enthalpy given above is taken from a table in Ref. 1. The values in that table were chosen to agree with the α -phase data of Ginnings and Corruccini²⁸ and to reproduce measured enthalpy increments for the β and γ phases.

Table 4. Temperature Range of Enthalpy and Heat Capacity Measurements for Uranium

Temperature Range, K	Experimenter	Ref.
298-1300	Moore and Kelley	27
298-1178	Ginnings and Corruccini	28
373-1073	North	29
413-1454	Savage and Seibel	30
323-873	Mit'kina	31
1205-1579	Levinson	32
1428-2348	Stephens	33

Heat of Fusion, ΔH_m : 9.1 kJ/mol

This value is based on an experiment by Stephens³³ which gave a value of 9.142 kJ/mol for the heat of fusion. Levinson³² measured the heat of fusion to be (8.326 ± 0.544) kJ/mol. The value by Stephens was selected¹ because of the extensive range of his experiments 1428-2348 K and because he avoided problems of contamination by using levitation calorimetry.

Enthalpy, $H_{(BP)} - H_{(298)}$: 205.0 kJ/mol

This value is from tabulated values of enthalpy given in Ref. 1. Enthalpy experiments have been performed to 2348 K by Stephens.³³ The equation given by Stephens to fit his data in the temperature range 1728-2348K (converted to SI units) is

$$H_T - H_{(298)} \text{ (J/mol)} = 48.66 T - 1.014 \times 10^4$$

Heat of Vaporization, $\Delta H_{V(298)}$: 531^{+8}_{-4} kJ/mol

The value 531^{+8}_{-4} kJ/mol for the heat of vaporization at 298 K is the value recommended by the IAEA Panel on the uranium-plutonium carbide system. It is recommended in Ref. 1 as being the value most compatible with all the data on uranium systems. Many experiments on uranium vapor pressure have been performed, with the highest temperature (2500 K) being investigated by Ackermann and Rauh.²² Table 5 gives the value of the heat of vaporization at 0 and 298 K from the various experiments.

Table 5. Heat of Vaporization of Uranium

ΔH_V , kJ/mol	T, K	Experimenter	Year	Ref.
487.8 $\pm$ 0.4	0	Rauh and Thorn	1954	34
527 $\pm$ 21	0	DeMaria <i>et al.</i>	1960	35
487.4	298	Alcock and Grieseson	1961-1962	36
525.1 $\pm$ 10.5	298	Drowart <i>et al.</i>	1965	37
517.6 $\pm$ 5.4	298	Leitnaker and Godfrey	1967	38
529.3	298	Storms	1967	39
537.6 $\pm$ 8	298	Pattoret <i>et al.</i>	1968	40
539.7 $\pm$ 8	298	Pattoret <i>et al.</i>	1969	41
528.4 $\pm$ 4.2	298	Ackermann <i>et al.</i>	1961	42
530.1	298	Ackermann and Rauh	1972	43
536 $\pm$ 8	298	Oetting and Leitnaker	1972	44

Heat Capacity, $C_{P(298)}$: 27.66 J/K.mol

This value, from Ref. 1, is based on the heat capacity measurements of Flowtow and Lohr⁴⁵ and those of Flowtow and Osborne.⁴⁶

Heat Capacity, $C_p^{(s)}$: 38.28 J/K·mol
 $C_p^{(MP)}$

The value for the heat capacity of solid uranium at the melting point is that recommended in Ref. 1. It is the constant value of heat capacity for the γ phase determined from experiments of Ginnings and Corruccini.²⁸ Table 6 gives the reported values for heat capacity of the γ phase of uranium.

Table 6. Heat Capacity of the γ Phase of Uranium

C_p (γ -phase) J/K·mol	Experimenter	Ref.
38.07	Moore and Kelley	27
38.28	Ginnings and Corruccini	28
40.08	Levinson	32

Heat Capacity, $C_p^{(l)}$: 48.66 J/K·mol
 $C_p^{(MP)}$

The recommended¹ heat capacity of liquid uranium at the melting point is the constant value for liquid uranium from experiments of Stephens.³³

Thermal Conductivity, $K_{(298)}$: 27.6 W/m·K

This is the value recommended by Touloukian.¹³ It is based on his analysis of 109 sets of measurements by 36 experiments from 2.5 K^{46a} to 1173 K.^{46b}

Density, $\rho^{(s)}$: 1.90×10^4 kg/m³
 $\rho_{(298)}$

The value of density of uranium at 298 K is that recommended by the Joint Committee on Powder Diffraction Patterns.⁴⁷

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}^{(s)}$: 6×10^{-5} K⁻¹ (α phase)
 5×10^{-5} K⁻¹ (β phase)
 7×10^{-5} K⁻¹ (γ phase)
 $\bar{\alpha}_{(298-MP)}$

There are the values recommended by Touloukian,¹³ who analyzed data from 0 to 1373 K⁴⁸ from 48 experiments.

Temperature of Phase Transitions: $\alpha \rightarrow \beta$, 940.9 ± 1 K
 $\beta \rightarrow \gamma$, 1048.0 ± 1.6 K

These values are taken from experiments by Blumenthal.²³ Although many investigators have reported values for these transitions, their data are often uncertain because of impurities in their samples or undercooling effects, or because the primary purpose of the experiment was not the phase transition temperature. Blumenthal's values are believed the most reliable because he did a careful study using high-purity electrolytic uranium and circumvented the problems of hysteresis, superheating, and undercooling.¹

THORIA (ThO₂)

Melting Point: 3643 ± 30 K

The value 3643 ± 30 K is recommended by Rand² and based on the following experimental information. Benz⁴⁹ recommends, in his phase diagram, a value of 3663 K for the melting point of ThO₂. Experiments by Lambertson *et al.*⁵⁰ on the ThO₂-UO₂ system gave melting points for ThO₂ ranging from 3558 to 3828 K, a result of variable contamination from the container. When these results were extrapolated to pure thoria, a value of 3623 K was obtained. However, Lambertson recommended a somewhat lower value, 3573 K, for the melting point to allow for curvature in the ThO₂ end of the system as was found with UO₂. However, this curvature in the UO₂ system is believed due to excess oxygen and thus would not occur in the ThO₂ system. Rand therefore gave greater weight to the higher values.

Boiling Point: 4320 K

The boiling point was calculated by us from extrapolated vapor-pressure data. The maximum temperature of vapor-pressure experiments is 2800 K.⁵¹

Enthalpy, H_(MP) - H₍₂₉₈₎: 290.4 kJ/mol

The values given in Ref. 2 (p. 35, Table 7) for the heat capacity were used by us to extrapolate to the melting point. From those values, the enthalpy to the melting point was calculated. Experimental enthalpy data are available up to 2773 K.⁵²

Heat of Fusion, ΔH_m: 90.8 kJ/mol

This value was calculated by us assuming that the heat of fusion = nR, where n is the number of atoms per molecule of the compound. However, the value may be too low if the heat capacity of the ThO₂ does not increase as melting is approached, as does the heat capacity of UO₂. See Fig. 2 in the appendix.

Enthalpy, H_(RP) - H₍₂₉₈₎: 484.1 kJ/mol

This value was calculated by us using H_(MP) - H₍₂₉₈₎ and the heat of fusion value (given above) and then extrapolating to the boiling point using our estimated value for the heat capacity of liquid ThO₂.

Heat of Vaporization, ΔH_v(298): 664.0 ± 10.5 kJ/mol

This value, recommended in Ref. 3, is from experiments by Ackermann *et al.*⁵³ Tabulated below are the available values of heat of vaporization at 298 K derived from the temperature dependence of vapor pressure measurements.

Table 7. Heat of Vaporization of ThO₂

ΔH_V (298) kJ/mol	Temperature Range of Experiments, K	Experimenter	Ref.
664.0 $\pm$ 10.5	2180-2865	Ackermann <i>et al.</i>	53
715	2050-2250	Shapiro	54
712.5	2398-2677	Hoch and Johnston	55
770	2040-2320	Fan	56

Heat Capacity, C_P (298) : 61.73 J/K·mol

The heat capacity data for thoria are very consistent. The recommended² value for C_P is taken from experiments by Osborne and Westrum,⁵⁷ who measured heat capacity from 10 to 305 K. It also agrees exactly with the value calculated from an equation given by Godfrey *et al.*⁵⁹ to fit the data of Osborne and Westrum,⁵⁷ Victor and Douglas^{58a} (323-1173) K, Southard^{58b} (522-1786 K), and Hoch and Johnston⁵² (1456-2753 K). This equation, converted to SI units, is

$$C_P \text{ (J/K·mol)} = 69.29 + 9.339 \times 10^{-3} T - 9.184 \times 10^{-5} T^{-2} \quad (9)$$

for the temperature range 298 to 3000 K.

Heat Capacity, C_P (s) : 103.2 J/K·mol
(MP)

Heat capacity and enthalpy measurements for ThO₂ have been performed only to 2773 K.⁵² In the regions of experimental overlap, there is excellent agreement. By fitting the available experimental data, Godfrey *et al.*⁵⁸ obtained Eq. 9, as described above. The above value for heat capacity at the melting point (103.4 J/K·mol) was found by extrapolating to the melting point the values of heat capacity given in Ref. 2 (p. 35, Table 7). The tabulated values are represented by Eq. 9.

Heat Capacity, C_P (l) : 136.0 J/K·mol
(MP)

No data exist. The value is assumed to be equal to that of UO₂.

Heat Capacity, C_P (l) : 136.0 J/K·mol
(BP)

No data exist. The value is assumed to be equal to that of UO₂ measured at lower temperatures.

Thermal Conductivity, $K_{(298)}$: 13.2 W/m·K

This value is recommended by Touloukian.¹³ It is based on 10 sets of data by seven authors. The temperatures of measurements range from 304 K⁵⁹ to 2009 K.⁶⁰

Density, $\rho_{(298)}^{(s)}$: $(1.0013 \pm 0.0001) \times 10^4 \text{ kg/m}^3$

This value, from Ref. 2 (Table XXIV on page 199), is based on the lattice parameters of Skinner.⁶¹

Density, $\rho_{(MP)}^{(s)}$: $8.8 \times 10^3 \text{ kg/m}^3$

This is an extrapolated value.³ The maximum temperature of experiments is 2700 K.⁶²

Change in Density on Melting, $\left(-\frac{\Delta\rho}{\rho}\right)_{MP}$: 0.11

No data exist. The value is assumed equal to that of UO₂.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}^{(s)}$: $3.5 \times 10^{-5} \text{ K}^{-1}$

This value is from thermal expansion measurements by Hoch and Momin.^{62a} Their equation for percent linear thermal expansion for solid ThO₂ is

$$(100\%) \times \frac{(L_T - L_{25})}{L_T} = 8.383 \times 10^{-4} T + 0.995 \times 10^{-7} T^2 - 2.106 \times 10^{-2} \quad (10)$$

where T is given in °C.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(MP)}^{(l)}$: $9 \times 10^{-5} \text{ K}^{-1}$

No data exist. The value is assumed equal to that of UO₂.

Viscosity, $\eta_{(MP)}$: $(4.30 \pm 0.10) \times 10^{-3} \text{ Pa}\cdot\text{s}$

No data exist. The value is assumed equal to that of UO₂.

THORIUM-URANIUM OXIDE $[(\text{Th}_{0.9}\text{U}_{0.1})\text{O}_2]$ Melting Point: 3500 K

This value was taken by us from a plot³ of melting point *vs.* composition for stoichiometric $(\text{Th},\text{U})\text{O}_2$ from data from experiments of Lambertson *et al.*⁶³ and Christensen.⁶⁴

Boiling Point: 4250 K

The maximum temperature of reported vapor pressure experiments is 2800 K.⁵¹ The boiling point was calculated by us from extrapolated vapor pressure data. The vapor pressure values were corrected using the heat of vaporization obtained from our estimated heat of fusion at the melting point. The boiling point was taken as the temperature at which the vapor pressure equals 1 atm. The equation used to determine the total pressure from the partial pressures, previously presented as Eq. 5, is as follows:

$$P = \sum_i P_i X_i$$

where

P_i = the pressure of the i^{th} component

X_i = the mole fraction of the i^{th} component

Enthalpy, $H_{(\text{MP})} - H_{(298)}$: 265.6 kJ/mol

Experimental enthalpy data exist only to 2270 K.⁶⁵ The value given above was calculated by us. An estimate of the enthalpy at the melting point was obtained by applying the enthalpy equation formulated by Springer *et al.*⁶⁵ to fit their experimental data from 273 K through 2270 K:

$$H_{(\text{T})} - H_{(298)} \text{ (J/mol)} = -2.3502 \times 10^4 + 69.96T \\ + 35.925 \times 10^{-4} T^2 + 6.957 \times 10^5 T^{-1}$$

where T is temperature K. For comparison, a molar average of the ThO_2 and UO_2 enthalpy differences gives a value of 291.2 kJ/mol; therefore, the estimate appears reasonable.

Heat of Fusion, ΔH_m : 87.4 kJ/mol

This value is a calculated molar average. No data exist for $\text{Th}_{0.9}\text{U}_{0.1}\text{O}_2$.

Enthalpy, $H_{(\text{BP})} - H_{(298)}$: 471.1 kJ/mol

This value is a calculated molar average. Enthalpy measurements for $\text{Th}_{0.9}\text{U}_{0.1}\text{O}_2$ have been made only to 2270 K.⁶⁵

Heat of Vaporization, ΔH_V : 602 kJ/mol
(298)

The heat of vaporization was determined from the slope of the $\ln P$ vs. $1/T$ curve where P = pressure and T = temperature. The maximum temperature of the vapor pressure data is 2800 K.⁵¹

Heat Capacity, C_P : 64.27 J/K·mol
(298)

This value was calculated from the equation

$$C_P = 69.96 + 7.185 \times 10^{-3} T - 6.957 \times 10^{-5} T^2 \quad (\text{J/K}\cdot\text{mol}) \quad (12)$$

where T is temperature in degree Kelvin. The equation was derived by Springer *et al.*⁸⁵ by a least squares fit of their experimental enthalpy data from 273 to 2270 K.

Heat Capacity, $C_P^{(s)}$: 93 J/K·mol
(MP)

This value was estimated by extrapolating the data of Springer *et al.*⁸⁵ to the melting point, using Eq. 12, given above. For comparison, a molar average of the heat capacities of ThO_2 and UO_2 gives 113.8 J/K·mol; therefore, extrapolation appears reasonable.

Heat Capacity, $C_P^{(l)}$: 136.0 J/K·mol
(MP)

No data exist for ThO_2 or for $\text{Th}_{0.9}\text{U}_{0.1}\text{O}_2$. The value is assumed equal to that of UO_2 .

Heat Capacity, $C_P^{(l)}$: 136.0 J/K·mol
(BP)

No data exist for ThO_2 or for $\text{Th}_{0.9}\text{U}_{0.1}\text{O}_2$. The value is assumed equal to that of UO_2 .

Thermal Conductivity, $K_{(298)}$: 11.1 W/m·K

This value was obtained for $(\text{Th}_{0.9}\text{U}_{0.1})\text{O}_2$ of 100% theoretical density, from the equation

$$K \text{ (W/m}\cdot\text{K)} = \left[\frac{(1 - P)(0.67 + 0.282U)}{0.67 + 0.282U + P(1 + 0.092U)} \right] \times \left[\frac{1}{0.79(1 + 0.09U) + 0.0185T} \right] \left(\frac{1 + 0.291U}{1 + 0.400U} \right) \times 10^2 \quad (13)$$

where P = the fractional porosity and U = the weight percent of UO₂; this equation was derived by Springer *et al.*⁶⁵ to fit their experimental data from 500-2200 K. The thermal conductivity of (Th,U)O₂ is sensitive to sample preparation and composition. Below 1300 K, there is wide variation in the data.³ Below 500 K, reported experimental values differ by as much as a factor of 10.

Density, $\rho_{(298)}^{(s)}$: $1.009 \times 10^4 \text{ kg/m}^3$

The value given here, recommended in Ref. 3, is from measurements by Cohen and Berman.⁶⁶ Variations exist among reported values of lattice parameters and densities for (Th,U)O₂. These discrepancies are probably due to variations in purity or stoichiometry.

Density, $\rho_{(MP)}^{(s)}$: $8.8 \times 10^3 \text{ kg/m}^3$

The value is assumed equal to the value for ThO₂. No data exist.

Change in Density on Melting, $\left(-\frac{\Delta\rho}{\rho}\right)_{MP}$: 0.11

No data exist for ThO₂ or for the mixed oxide. The value is assumed equal to that of UO₂.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(298-MP)}^{(s)}$: $3.5 \times 10^{-5} \text{ K}^{-1}$

The value is assumed equal to that for ThO₂. The thermal expansion of Th_{0.9}U_{0.1}O₂ has been determined to 2270 K by Springer *et al.*⁶⁵ In the region from 298 K to 2270 K, the thermal expansion coefficient of Th_{0.9}U_{0.1}O₂ is quite close to that of ThO₂. At 2270 K, it differs by less than 3%. The difference in thermal expansion decreases as the temperature increases.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(MP)}^{(l)}$: $9 \times 10^{-5} \text{ K}^{-1}$

No data exist for the mixed oxide or for ThO₂. The value is assumed equal to that of UO₂.

Viscosity, $\nu_{(MP)}$: $(4.30 \pm 0.10) \times 10^{-3} \text{ Pa}\cdot\text{s}$

No data exist for the mixed oxide or for ThO₂. The value is assumed equal to that of UO₂.

URANIA (UO₂)

Melting Point: 3138 ± 15 K

This value based on experiments of Latta and Fryxell⁶⁷ has been recommended by Leibowitz *et al.*⁴ because it is the most recent and most accurate of thermal arrest measurements. It agrees within experimental error with earlier experiments of Lyon and Bailey.⁶⁸

Boiling Point: 3760 ± 200 K

This value was calculated by Leibowitz *et al.*⁴ from vapor pressure data. Experiments have been performed to 3500 K.⁶⁹

Enthalpy, H_(MP) - H₍₂₉₈₎: 310.0 kJ/mol

The value was taken from tabulated enthalpy values in Ref. 4. It is based on the equation (which we have converted to SI units)

$$\Delta H_{(298)} \text{ (J/mol)} = K_1 \theta [e^{\theta/T} - 1]^{-1} - (e^{\theta/298} - 1)^{-1} \\ + K_2 [T^2 - (298)^2] + K_3 e^{-E_D/RT} \quad (14)$$

where

T = temperature, in K from 298-3137 K

θ = 535 K

E_D = 157.69 kJ/mol

K₁ = 80.08 J/mol·K

K₂ = 3.28 × 10⁻³ J/mol·K²

K₃ = 2.36 × 10⁷ J/mol

derived by Kerrisk and Clifton⁷⁰ to fit the most reliable UO₂ enthalpy data.^{27,71-74}

Heat of Fusion, ΔH_m: 74.9 ± 1.2 kJ/mol

This is an average value⁴ from measurements of Chikalla,⁷⁵ Leibowitz *et al.*,⁷³ and Hein and Flagella.⁷⁶ All three experimental values agree within experimental error.

Enthalpy, H_(BP) - H₍₂₉₈₎: 469.4 kJ/mol⁴

This value is extrapolated by us from tabulated enthalpy values in Ref. 4. Experimental measurements go to 3500 K.⁷³

Heat of Vaporization, $\Delta H_{V(298)}$: 598 kJ/mol

This value is from experimental data of Tetenbaum and Hunt.⁷⁷

Heat of Vaporization, $\Delta H_{V(BP)}$: 454 ± 53 kJ/mol

This value, recommended by Leibowitz *et al.*,⁴ is based on UO₂ vapor pressure-temperature data. Experiments go to 3500 K.⁶⁹

Heat Capacity, $C_{P(298)}$: 63.6 J/K·mol

This value is highly recommended by Leibowitz *et al.*⁴ It is calculated from an equation of Kerrisk and Clifton⁷⁰ and is also in good agreement with the most reliable experimental data.^{27,71-74}

Heat Capacity, $C_{P(MP)}^{(s)}$: 208.4 J/K·mol

This value is from tabulated heat capacities given in Ref. 4. It is calculated from the following equation (which we have converted to SI units), derived by Kerrisk and Clifton⁷⁰ from enthalpy data:^{27,71-74}

$$C_p = \frac{K_1 \theta^2 e^{\theta/T}}{T^2 (e^{\theta/T} - 1)^2} + 2K_2 T + \frac{K_3 E_D}{RT^2} e^{-E_D/RT} \quad (15)$$

where

T = temperature in K from 298-3137 K

$\theta = 535$ K

$E_D = 157.69$ kJ/mol

$K_1 = 80.08$ J/mol·K

$K_2 = 3.28 \times 10^{-3}$ J/mol·K²

$K_3 = 2.36 \times 10^7$ J/mol

Heat Capacity, $C_{P(MP)}^{(l)}$: 136.0 J/K·mol

This value, given in Ref. 4, is from experimental enthalpy data for liquid UO₂ by Leibowitz *et al.*⁷⁸ The enthalpy data of Hcin and Flagella⁷⁶ for liquid UO₂ is in good agreement.

Heat Capacity, $C_P^{(l)}$: 136.0 J/mol·K
(BP)

This value, recommended by Leibowitz *et al.*,⁴ is extrapolated from experimental enthalpy data for liquid UO₂ to 3500 K by Leibowitz *et al.*⁷⁸ The enthalpy data of Hein and Flagella⁷⁶ are in good agreement.

Thermal Conductivity, $K_{(298)}$: 8.4 W/m·K

This value recommended by the 1964 IAEA Panel⁷⁹ is based on measurements by Penninckx⁸⁰ on single crystal UO₂ from 4 to 300 K. Measurements were also made in the same temperature range by Bethaux *et al.*⁸¹ on sintered polycrystalline UO₂.

Normal Spectral Emissivity, $\epsilon_{(0.65 \mu m)}$: 0.87 ± 0.1

This value of normal spectral emissivity 0.65 μm , recommended by Leibowitz *et al.*,⁴ is from experiments by Held and Wilder⁸² from 450 to 2400 K. It agrees well with the data of Cabannes *et al.*⁸³ but disagrees with the results of Claudson.⁸⁴ Claudson's data indicated a decrease in emissivity from 1000 to 2220 K, whereas the more recent experiments of Held and Wilder show little sensitivity to temperature.

Density, $\rho_{(298)}^{(s)}$: 1.097 x 10⁴ kg/m³

The theoretical density of UO₂ recommended by Leibowitz *et al.*⁴ is from the measurements of Swanson and Fuyat.⁸⁵

Density, $\rho_{(MP)}^{(s)}$: 9.71 x 10³ kg/m³

This value was calculated by Leibowitz *et al.*⁴ via the equation:

$$\rho(\text{kg/m}^3) = (1.097 \times 10^4)[1 + 2.04 \times 10^{-5}(T - 273) + 8.7 \times 10^{-9}(T - 273)^2]^{-1} \quad (16)$$

This equation is based on experiments in the temperature range 298 K to 3137 K. The results of this equation agree withing ±2% with the high temperature values reported by Christensen.⁸⁶

Change of Density on Melting, $\left(-\frac{\Delta\rho}{\rho}\right)_{MP}$: 0.11

This value is calculated from tabulated density values by Leibowitz *et al.*⁴

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(298-MP)}^{(s)}$: 4.5 x 10⁻⁵ K⁻¹

This value for the volumetric expansion coefficient is calculated from the linear expansion coefficient obtained from an equation given in Ref. 4.

$$\alpha(\text{linear}) (\text{K}^{-1}) = 6.8 \times 10^{-6} + 2.9 \times 10^{-9}(T - 273) \quad (17)$$

The results of this equation give good agreement with the data from experiments of Conway *et al.*⁸⁷ and that of Christensen⁸⁶ to the melting point.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(MP)}^{(l)}$: $9 \times 10^{-5} \text{ K}^{-1}$

This value was calculated from the mean linear expansion coefficient for liquid UO₂ given by Leibowitz *et al.*⁴ It is based on the results of thermal expansion data for liquid UO₂ by Christensen.⁸⁶

Viscosity, $\nu_{(MP)}$: $(4.30 \pm 0.10) \times 10^{-3} \text{ Pa}\cdot\text{s}$

This is the value tabulated by Leibowitz *et al.*⁴ It is based on experiments by Woodley.⁸⁸ The experiments of Tsai and Olander⁸⁹ give slightly higher values, but confirm the magnitude of the values of Woodley.

Surface Tension, σ : $0.45 \pm 0.04 \text{ N/m}$

This value is recommended by Leibowitz *et al.*⁴ It is an average of three different measurements by Chasanov *et al.*⁹⁰

URANIUM-PLUTONIUM OXIDE [(U_{0.8}Pu_{0.2})O₂]

Melting Point: 3063 K liquidus
 3023 K solidus

These values were calculated by Leibowitz *et al.*⁴ They are in good agreement with experimental data of Lyon and Bailey⁶⁸ and those of Aitken and Evans.⁹¹

Boiling Point: 3520 K

The boiling point of 3520 K was calculated by Leibowitz *et al.*⁴ from vapor pressure data. Although vapor pressure experiments have been performed to 7000 K,^{92,94-95} questions exist concerning proper interpretation of the high temperature data obtained by laser-evaporation experiments. Therefore, vapor pressures from calculations of Breitung,⁹³ based on experiments to 2400 K,⁹⁴⁻⁹⁵ were used.

Enthalpy, H_(MP) - H₍₂₉₈₎: 282.5 kJ/mol

This value is for the solidus temperature (3023 K) and is from tabulated enthalpy values by Leibowitz *et al.*⁴ The tabulated values of enthalpy differences in the solid range were calculated by an equation derived by Gibby *et al.*⁹⁶ to fit most reliable enthalpy data.⁹⁷⁻⁹⁹ The equation, which is applicable for T = 298-3000 K is as follows:

$$\begin{aligned} H_T - H_{(298)} \text{ (J/mol)} &= -1.839 \times 10^4 + 52.47 T + 3.56 \times 10^{-2} T^2 \\ &\quad - 1.63 \times 10^{-5} T^3 + 3.20 \times 10^{-9} T^4 \end{aligned} \quad (18)$$

Heat of Fusion, ΔH_m: 74.9 ± 1.2 kJ/mol

This is the value recommended by Leibowitz *et al.*⁴ It is the same as that for UO₂. Only one measurement of the heat of fusion of the mixed oxide has been made,¹⁰⁰ and this value, 67.4 kJ/mol, is within 10% of the value for UO₂. Thus, Leibowitz *et al.*¹⁰⁰ recommend that the value for UO₂ be used until more data are available.

Enthalpy, H_(BP) - H₍₂₉₈₎: 425.5 kJ/mol

The value was obtained from extrapolation of tabulated enthalpies in Ref. 4. Experimental enthalpy data go to 3000 K.¹⁰⁰

Heat of Vaporization, ΔH_V (298): 619 kJ/mol

The heat of vaporization was found from the slope of the log of the vapor pressure *vs.* inverse temperature curve and applying the Clausius-Claperyon equation.⁴

Heat of Vaporization, ΔH_V : 536 $\pm$ 54 kJ/mol
(BP)

The heat of vaporization was calculated from vapor pressure data.⁴ Although experimental measurements have been made to 7000 K,⁹² questions exist concerning the proper interpretation of the high temperature data obtained by laser-evaporation experiments. Thus, vapor pressure calculations of Breitung⁹³ based on experiments to 2400 K⁹⁴⁻⁹⁵ were used.

Heat Capacity, $C_{P(298)}$: 69.6 J/K·mol

The value is from tabulated heat capacity values given in Ref. 4. It was calculated from an equation derived by Gibby *et al.*,⁹⁶ to fit the most reliable enthalpy data.⁹⁷⁻⁹⁹ This equation is:

$$C_p \text{ (J/K·mol)} = 52.47 + 7.1 \times 10^{-2}T - 4.90 \times 10^{-5} T^2 + 1.28 \times 10^{-8} T^3 \quad (19)$$

where T is in K. The only direct measurements of heat capacities were made by Affortit and Marcon.¹⁰¹

Heat Capacity, $C_{P(MP)}^{(s)}$: 173.3 J/K·mol

This value for the heat capacity of the solidus was calculated from Eq. 19 given above for $C_{P(298)}$.

Heat Capacity, $C_{P(MP)}^{(l)}$: 136.0 J/K·mol

The heat capacity value for liquid U_{0.8}Pu_{0.2}O₂ recommended in Ref. 4 is from enthalpy experiments by Leibowitz *et al.*¹⁰⁰ Their experimental values agreed with the established values for UO₂ within 10%, therefore, the experimenters recommended using the values for molten UO₂ until more data are available.

Heat Capacity, $C_{P(BP)}^{(l)}$: 136.0 J/K·mol

No data exist for U_{0.8}Pu_{0.2}O₂. The value is assumed equal to that for UO₂.

Thermal Conductivity, $K_{(298)}$: 6.3 W/m·K

The value is from measurements by Seddon.^{102,103}

Normal Spectral Emissivity, $\epsilon_{(0.65 \mu m)}$: 0.87 $\pm$ 0.1

This value is recommended by Leibowitz *et al.*⁴ for the temperature range from 450 to 2400 K, since no emissivity data for UO₂-PuO₂ have been reported. The value is due to emissivity data for UO₂ by Held and Wilder.⁸²

Density, $\rho_{(298)}^{(s)}$: 1.108 $\times$ 10⁴ kg/m³

This value is from Ref. 4. The density of mixed (U,Pu) oxides has not been directly measured as a function of temperature. It is a function of ²³⁵U

enrichment, Pu content, Pu isotopes, and O/M.⁴ The equation given in Ref. 4 to calculate the theoretical density is

$$\rho \text{ (kg/m}^3\text{)} = 6.64046 \times 10^3 \frac{[\bar{M}_U + Y(\bar{M}_{Pu} - \bar{M}_U) + 16 X]}{(6.1127 - 0.534 Y - 0.321 X + 0.229 XY)^3} \quad (20)$$

where

$\bar{M}_U$ = average molecular weight of uranium

$\bar{M}_{Pu}$ = average molecular weight of plutonium

$X = O/M$

$Y = Pu/(U + Pu)$

X and Y = lattice parameter correlations of Schnizlein¹⁰³

Density, ρ ^(s)_(MP): $9.88 \times 10^3 \text{ kg/m}^3$

The value is from Ref. 4. Leibowitz *et al.* calculated density as a function of temperature from the equation

$$\rho \text{ (kg/m}^3\text{)} = 1.108 \times 10^4 [1 + 2.04 \times 10^{-5}(T - 273) + 8.7 \times 10^{-9}(T - 273)^2]^{-1} \quad (21)$$

where T is in K in the range $273 \leq T \leq 2998$. No density measurements as a function of temperature have been made.

Change in Density on Melting, $\left(-\frac{\Delta\rho}{\rho}\right)_{MP}$: 0.11

This value is from thermal expansion recommendations of Ref. 4. No data exist for the thermal expansion of (U,Pu)O₂ above the melting point. However, since the thermal expansion data for solid (U,Pu)O₂ indicate that the presence of Pu has little effect, the thermal expansion of molten UO₂ from measurements of Christensen⁸⁶ is used for (U,Pu)O₂. Thus the fractional change in density at the melting point for U_{0.8}Pu_{0.2}O₂ is taken to be equal to that of UO₂. Because (U,Pu)O₂ does not have a sharp melting point, the density change is spread over the temperature region between the solidus (3023 K) and the liquidus (3063 K).

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}$ ^(s)_(298-MP): $4.5 \times 10^{-5} \text{ K}^{-1}$

Thermal expansion data for UO₂,^{86,87} PuO₂,^{105,106} and U_{0.75}Pu_{0.25}O₂^{107,110} indicate that the presence of Pu has negligible effect on thermal expansion in UO₂-PuO₂ solid solutions. Thus, the thermal expansion is taken to be equal to that of UO₂.⁴

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(MP)}^{(l)}$: $9 \times 10^{-5} \text{ K}^{-1}$

There are no data reported for the thermal expansion of liquid $(U,Pu)O_2$. Since the thermal expansion below its melting point is identical to UO_2 , Leibowitz *et al.*⁴ recommended using the value for liquid UO_2 of Christensen.⁸⁶

Viscosity, $\nu_{(MP)}$: $(4.30 \pm 0.10) \times 10^{-3} \text{ Pa}\cdot\text{s}$

No measurements of the viscosity of $(U_{0.8}Pu_{0.2})O_2$ have been made. Thus Leibowitz *et al.*⁴ recommend using the value for UO_2 from experiments by Woodley.⁸⁸

Surface Tension, σ : $0.45 \pm 0.04 \text{ N/m}$

The surface tension of $(U,Pu)O_2$ has not been determined. Therefore, Leibowitz *et al.*⁴ recommend using the value for UO_2 from three measurements by Chasanov *et al.*⁹⁰

THORIUM CARBIDE (ThC)

Melting Point: 2773 ± 35 K

This value, recommended by Rand,² is from experiments of Benz and Stone¹¹¹ and those of Henney and Jones.¹¹² Wilhelm and Chiotti¹¹³ obtained a higher value of 2898 ± 25 K.

Enthalpy, $H_{(MP)} - H_{(298)}$: 155.2 kJ/mol

This is an estimate made by Schick.¹¹⁴ Apparently, no experimental enthalpy data exist.

Heat of Fusion, ΔH_m : 46 kJ/mol

No experimental data exist. This value was calculated assuming that the entropy of fusion = nR , where n equals the number of atoms per molecule of the compound.

Heat Capacity, $C_{P(298)}$: 45.2 ± 0.4 J/K·mol

This value, recommended by Rand,² is from heat capacity measurements from 5 to 300 K by Danan.¹¹⁵ The only other measurements have been by Harness *et al.* from 1.8 to 4.2 K.¹¹⁶

Heat Capacity, $C_{P(MP)}^{(s)}$: 73.6 J/K·mol

This is an estimate made by Schick.¹¹⁴ Apparently no experimental data exist.

Heat Capacity, $C_{P(MP)}^{(l)}$: 71 J/K·mol

No data exist. The value is assumed to be equal to that of UC.

Thermal Conductivity, $K_{(298)}$: 12 W/m·K

No data on the thermal conductivity of ThC exist. The value is assumed to be equal to that for $Th_{0.9}U_{0.1}C$.

Density, $\rho_{(298)}^{(s)}$: 1.061×10^4 kg/m³

The value of the density is that recommended by the Joint Committee on Powder Diffraction Patterns.¹¹⁷

Density, ρ ^(s)_(MP): $1.02 \times 10^4 \text{ kg/m}^3$

This value was calculated by us from thermal expansion coefficients given by Peterson and Curtis in Ref. 3.

Volumetric Expansion Coefficient, $\bar{\alpha}$ ^(s)_(298-MP): $1.7 \times 10^{-5} \text{ K}^{-1}$

This value is extrapolated from experimental data below 1300 K. The existing data collected in Ref. 3 and the average linear expansion coefficients (when available) for that range are tabulated below.

Table 8. Measurements of the Average Coefficient of Linear Expansion

$\bar{\alpha}$ Linear, $10^{-6}/\text{K}$	Temperature Range, K	Experimenter	Ref.
6.53 ± 0.071	291-1114	Street and Water	118
4.6	298-1273	Chiotti and White	119
8.5 ^a	973-1700	Satow	120
-	1173-1700	Aronson <i>et al.</i>	121

^aThis value is for ThC_{0.96}.

THORIUM-URANIUM CARBIDE [(Th_{0.9}U_{0.1})C]Melting Point: 2775 K

No data exist. This is the calculated molar average.

Enthalpy, $H_{(MP)} - H_{(298)}$: 156.9 kJ/molNo data exist. This is the calculated molar average. Note that the value used for ThC in the molar average is an estimate made by Schick.¹¹⁴Heat of Fusion, ΔH_m : 46 kJ/molNo experimental data exist. This value was calculated assuming that the entropy of fusion = nR , where n is the number of gram atoms in the compound.Heat Capacity, $C_{P(298)}$: 45.6 J/K·mol

No data exist for the mixed monocarbide. This is the calculated molar average.

Heat Capacity, $C_{P(MP)}^{(s)}$: 74.9 J/K·molNo data exist. This is the calculated molar average. Note that the value used for ThC in the molar average is an estimate by Schick.¹¹⁴Heat Capacity, $C_{P(MP)}^{(l)}$: 71 J/K·mol

This value is assumed equal to that of UC. No data exist for either the mixed monocarbide or ThC.

Thermal Conductivity, $K_{(298)}$: 12 W/m·KThis value is from a compilation by Peterson *et al.*¹²² Measurements of the thermal conductivity of Th_{0.9}U_{0.1}C have been made only at 473 and 1073 K by Griesenauer *et al.*¹²³ The above value is an extrapolation from their data at 473 K.Density, $\rho_{(298)}^{(s)}$: 1.09×10^4 kg/m³This is a molar average calculated by us. No data exist for (Th_{0.9}U_{0.1})C.Density, $\rho_{(MP)}^{(s)}$: 1.04×10^4 kg/m³

This value was calculated by us from thermal expansion coefficients given by Peterson and Curtis in Ref. 3.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(298-MP)}^{(s)}$: 2.0×10^{-5} K⁻¹This value is based on measurements made by Griesenauer *et al.*¹²³ below 1300 K.³

URANIUM CARBIDE (UC)

Melting Point: 2780 ± 25 K

This is the value recommended by Johnson *et al.*¹²⁴

Boiling Point: 4800 K

This value was calculated by Sheth and Leibowitz from estimated vapor pressures.¹²⁵ Experimental vapor pressure data exist to 2480 K.¹²⁶

Critical Temperature: 9750 K

This is an estimate made by Sheth and Leibowitz.¹²⁵

Enthalpy, $H_{(MP)} - H_{(298)}$: 171.33 kJ/mol

This value is recommended by Storms and Ackermann.¹²⁷ The maximum temperature of the experimental data is 2480 K.¹²⁶

Heat of Fusion, ΔH_m : 46 kJ/mol

No data exist. This value was calculated assuming the heat of fusion = nR , where n is the number of atoms per molecule of the compound.

Enthalpy, $H_{(BP)} - H_{(298)}$: 372 kJ/mol

This value was calculated by Sheth and Leibowitz.¹²⁵ Experimental data go to 2481 K.¹²⁶

Heat of Vaporization, $\Delta H_{V(298)}$: 536 kJ/mol

This value is estimated by Johnson *et al.*¹²⁴ from the total vapor pressure assuming that the vapor is composed solely of UC.

Heat Capacity, $C_{P(298)}$: 50.2 J/K·mol

This value is recommended by Sheth and Leibowitz.¹²⁵ It is from the work of Tetenbaum *et al.*¹²⁶

Heat Capacity, $C_{P(MP)}^{(s)}$: 87.4 J/K·mol

This is the value recommended by Storms and Ackermann.¹²⁷ Experimental data exist to 2481 K.¹²⁶

Heat Capacity, $C_{P(MP)}^{(l)}$: 71 J/K·mol

This value was estimated by Sheth and Leibowitz.¹²⁵ No experimental data exist for the heat capacity of liquid UC.

Heat Capacity, $C_{P(BP)}^{(l)}$: 87.4 J/mol·K

This is an estimated heat capacity calculated by Sheth and Leibowitz.¹²⁵

Thermal Conductivity, $K_{(298)}$: 22 W/m·K

This is the value recommended by Johnson *et al.*¹²⁴ They recommend using equations which were derived to fit the data of Wheeler *et al.*¹²⁸ for thermal conductivity below 2573 K. These formulas are:

$$K \text{ (W/m·K)} = 0.228 \times 10^2 - 5.01 \times 10^{-3} T + 3.61 \times 10^{-6} T^2 \quad (22)$$

$$(323 < T < 973 \text{ K})$$

$$K \text{ (W/m·K)} = 19.8 + 1.48 \times 10^{-3} T \quad (23)$$

$$(973 < T < 2573 \text{ K})$$

where K is the thermal conductivity for UC of theoretical density. Correction for low-density material is made using the equation¹²⁴

$$K_{LD} = (1 - P)K$$

where

K = thermal conductivity of UC of 100% theoretical density

K_{LD} = thermal conductivity of low density material

P = the volume fraction porosity

Thermal Conductivity, $K_{(MP)}^{(s)}$: 24 W/m·K

This is an extrapolated value by Lewis and Kerrisk.¹²⁹ Experimental data go to 2573 K¹²⁸ and show a wide variation over the entire temperature range measured.

Thermal Conductivity, $K_{(MP)}^{(l)}$: 20 W/m·K

This is an estimate by Sheth and Leibowitz.¹²⁵ No experimental data exist on the thermal conductivity of liquid UC.

Normal Total Emissivity, ϵ_T : 0.42 ± 0.02

This is the value measured by Grossman¹³⁰ between 1250 and 1980 K and tentatively recommended by Sheth and Leibowitz.¹²⁵ It is lower than the emissivities of other refractory carbides and therefore may be too low. No other data exist.

Normal Spectral Emissivity, $\epsilon_{(0.65 \mu\text{m})}$: $0.539 - 2 \times 10^{-5} T$

This value, tentatively recommended by Sheth and Leibowitz,¹²⁵ was measured by Grossman¹³⁰ from 1150 K to 1890 K. Measurements of the normal spectral emissivity were also made by DeConinck.¹³¹ The value by Grossman appears to have the same temperature dependence as that of other refractory carbides, but it is lower. Thus it may be too low.

Density, $\rho_{(298)}^{(s)}$: $1.36 \times 10^4 \text{ kg/m}^3$

This value, recommended by Johnson *et al.*,¹²⁴ is from experiments of Mendez-Peñalosa and Taylor.^{131a}

Density, $\rho_{(MP)}^{(s)}$: $1.23 \times 10^4 \text{ kg/m}^3$

This value was calculated by us from the thermal expansion coefficients given by Sheth and Leibowitz.¹²⁵

Density, $\rho_{(BP)}^{(l)}$: $8.5 \times 10^3 \text{ kg/m}^3$

This value is an estimate from an equation derived by Sheth and Leibowitz:¹²⁵

$$\rho_L(\text{UC}) (\text{kg/m}^3) = \frac{1.257 \times 10^4}{1 + 9.98 \times 10^{-5} T} \quad (25)$$

where T (in kelvins) is equal to or greater than the melting point. No experimental data are available.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(298-MP)}^{(s)}$: $3.9 \times 10^{-5} \text{ K}^{-1}$

This value is based on the linear thermal expansion coefficient that was calculated by Sheth and Leibowitz.¹²⁵ They extrapolated the average linear thermal expansion coefficient from the measurements by Andrew¹³² to the melting point. Andrew's measurements range from room temperature to 2273 K.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(MP)}^{(l)}$: $8 \times 10^{-5} \text{ K}^{-1}$

This is an estimate by Sheth and Leibowitz.¹²⁵ There are no experimental data.

Isothermal Compressibility, $\kappa_{T(298)}$: $7.1 \times 10^{-12} \text{ Pa}^{-1}$

This value, recommended by Johnson *et al.*,¹²⁴ is due to Kempter.¹³³

Viscosity, $\nu_{(MP)}$: $8 \times 10^{-3} \text{ Pa}\cdot\text{s}$

This is an estimate made by Sheth and Leibowitz.¹²⁵ No data are available.

URANIUM-PLUTONIUM CARBIDE [(U_{0.8}Pu_{0.2})C]

Melting Point: 2780 K liquidus
2548 K solidus

These are the values of solidus and liquidus from experiments of Reavis, Johnson, and Leary.¹³⁵ Their results have been recommended by Fee and Johnson.¹³⁴

Boiling Point: 4560 K

This value was calculated by Sheth and Leibowitz¹²⁵ from calculated total vapor pressures as a function of temperature. No vapor pressure measurements have been made.

Critical Temperature: 9653 K

This is an estimate made by Sheth and Leibowitz.¹²⁵

Enthalpy, $H_{(MP)} - H_{(298)}$: 152.3 kJ/mol

This value is based on enthalpy measurements by D. F. Fischer from 1039 to 2421 K,¹³⁶ who derived an equation to fit his experimental data and the estimated enthalpy values¹²⁶ for lower temperatures. The equation is as follows:

$$H_T - H_{(298)} = -12.4866 \times 10^3 + 32.5225 T + 37.2021 \times 10^{-3} T^2 - 20.8151 \times 10^{-6} T^3 + 43.8487 \times 10^{-10} T^4 \quad (25)$$

where H is in joules per mole and T is in kelvins.

Heat of Fusion, ΔH_m : 45.6 kJ/mol

This was calculated by mole average from the calculated heats of fusion of UC (48.87 kJ/mol) and of PuC_{0.88} (37.97 kJ/mol).¹²⁵

Enthalpy, $H_{(BP)} - H_{(298)}$: 351.5 kJ/mol

This value was calculated by Sheth and Leibowitz.¹²⁵ Experimental enthalpy data exist to 2421 K.¹³⁶

Heat of Vaporization, $\Delta H_{V(298)}$: 536 kJ/mol

This value was calculated by Sheth and Leibowitz.¹²⁵ No data are available.

Heat Capacity, $C_{P(298)}$: 46.4 J/K·mol

This is the value for heat capacity recommended by Tetenbaum *et al.*¹²⁶

Heat Capacity, $C_{P(MP)}^{(s)}$: 106.8 J/K·mol

This value is an extrapolated value based on the enthalpy data of D. F. Fischer measured at 1039 to 2421 K.¹³⁶

Heat Capacity, $C_{P(MP)}^{(l)}$: 71 J/K·mol

This is an estimate made by Sheth and Leibowitz.¹²⁵ No experimental data are available.

Heat Capacity, $C_{P(BP)}^{(l)}$: 84.9 J/K·mol

This is an estimate made by Sheth and Leibowitz.¹²⁵ No data are available.

Thermal Conductivity, $K_{(298)}$: 17 W/m·K

This is the value recommended by Lewis and Kerrisk.¹²⁹

Thermal Conductivity, $K_{(MP)}^{(s)}$: 23 W/m·K

This value was extrapolated by Lewis and Kerrisk¹²⁹ from available experimental data to 573 K. Owing to inconsistencies in these data and the fact that some temperatures are not covered by experiments, a complete understanding of variations in thermal conductivity is lacking.

Thermal Conductivity, $K_{(MP)}^{(l)}$: 20 W/m·K

This is an estimate by Sheth and Leibowitz.¹²⁵ No experimental data exist on the thermal conductivity of liquid (U_{0.8}Pu_{0.2})C.

Density, $\rho_{(298)}^{(s)}$: 1.35×10^4 kg/m³

This value is recommended by Johnson *et al.*¹²⁴ It is based on two measurements by Andrew and Latimer¹³² which are tabulated in Table 9.

Table 9. Density Measurements of Andrew and Latimer¹³²

U Composition		Pu Composition		Measured Density, kg/m ³ (x10 ³)
²³⁵ U, %	²³⁸ U, %	²³⁹ Pu, %	²⁴⁰ Pu, %	
0.7	99.3	88-94	6-12	13.58 ± 0.01
93	7	88-94	6-12	13.46 ± 0.01

Density, $\rho_{(MP)}^{(s)}$: $1.23 \times 10^4 \text{ kg/m}^3$

This value was calculated by us based on thermal expansion coefficients given by Sheth and Leibowitz.¹²⁵

Density, $\rho_{(BP)}^{(l)}$: $8.6 \times 10^3 \text{ kg/m}^3$

This value is an estimate from an equation derived by Sheth and Leibowitz:¹²⁵

$$\rho_L = \frac{12.39 \times 10^3}{1 + 9.84 \times 10^{-5} T} \quad (\text{kg/m}^3) \quad (26)$$

where T (in K) is equal to or greater than the melting point. No experimental data are available.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(298-MP)}^{(s)}$: $3.4 \times 10^{-5} \text{ K}^{-1}$

This is an estimate made by Sheth and Leibowitz¹²⁵ based on the low-temperature data given by Andrew and Latimer.¹³²

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(MP)}^{(l)}$: $6.8 \times 10^{-5} \text{ K}^{-1}$

This is an estimate by Sheth and Leibowitz.¹²⁵ No experimental data exist.

Viscosity, $\nu_{(MP)}$: $7 \times 10^{-3} \text{ Pa}\cdot\text{s}$

This is an estimate made by Sheth and Leibowitz.¹²⁵ No data are available.

THORIUM DICARBIDE (ThC₂)Melting Point: 2913 ± 30 K

This is the value recommended by Fand.² It is close to the mean of two experimental measurements, namely, that of Benz and Stone¹¹¹ who found a melting point of 2883 ± 35 K, and that of Wilhelm and Chiotti¹¹³ who measured the melting point as 2938 ± 25 K.

Boiling Point: 5400 K

This is an extrapolated value.³

Enthalpy, H_(MP) - H₍₂₉₈₎: 218 kJ/mol

This value was estimated from data in Ref. 3 (p. 96, Table 19). However, that table is also based on estimates. The experimental data on enthalpy, which extend to about 1200 K, are inconsistent.

Heat of Fusion, ΔH_m: 71 kJ/mol

No experimental data are available. This value was calculated by assuming that the heat of fusion = nR, where n is the number of atoms per molecule of the compound.

Heat of Vaporization, ΔH_v: 690 kJ/mol

There is much controversy regarding the available vapor pressure data.³ Experimental data of Lonsdale and Graves¹³⁷ from 2278 to 2897 K are uncertain because of possible oxygen contamination in their ThC₂ source. Measurements by Jackson *et al.*¹³⁸ from 2371 to 2642 K give pressures lower by a factor of five. However, according to Storms,¹³⁹ the measurements of Kent¹⁴⁰ are close to the values of Lonsdale and Graves.

Heat Capacity, C_{p(298)}: 56.69 ± 0.59 J/K·mol

This value, recommended by Peterson and Curtis,³ is from experiments by Westrum *et al.*¹⁴¹ from 5 to 350 K. Measurements by Takahashi *et al.*¹⁴² for a near-stoichiometric specimen give 56.86 J/K·mol. An equation given by Rand² for the temperature range 298-1700 K gives 58.95 J/K·mol at 298 K. The equation is

$$C_p(\alpha \text{ phase})(\text{J/K}\cdot\text{mol}) = 65.69 + 1.209 \times 10^{-2} T - 9.25 \times 10^{-5} T^2 \quad (27)$$

Heat Capacity, C_{p(MP)}^(s): 83.6 J/K·mol

This value recommended by Rand² is an estimate by Holley and Storms.¹⁴³ No experimental data exist.

Density, $\rho_{(298)}^{(s)}$: $9.6 \times 10^3 \text{ kg/m}^3$

This is the value recommended by the Joint Committee on Powder Diffraction Patterns.¹⁴⁴

Density, $\rho_{(MP)}^{(s)}$: $9.0 \times 10^3 \text{ kg/m}^3$

This value was calculated by us from the thermal expansion coefficients given by Peterson and Curtis in Ref. 3.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(298-MP)}^{(s)}$: $7.8 \times 10^{-5} \text{ K}^{-1}$

This value, recommended by Peterson and Curtis,³ is from measurements of Langer *et al.*¹⁴⁵ to 2100 K. Measurements of the expansion of graphite-saturated ThC₂ were made by Cook¹⁴⁶ up to 1300 K.

Temperature of Phase Transitions: $\alpha \rightarrow \beta$, 1427 K
 $\beta \rightarrow \gamma$, 1490 K

These values are recommended values of Rand² based on eight experiments. The experimental values for the carbon-rich samples are tabulated in Table 10.

Table 10. Temperatures of the Phase Transitions of ThC₂

$T(\alpha \rightarrow \beta)$, K	$T(\beta \rightarrow \gamma)$, K	Experimenter	Ref.
1713	1768	Benz and Stone	111
1703 ± 10	1773 ± 25	Cook	146
1643 ± 15	1743 ± 15	Chiotti and White	119
1683	1749	Dolton <i>et al.</i>	147
1683 ± 20	1773 ± 20	Henney and Jones	112
1688 ± 10	1773	Hill and Cavin	148
1703	1763	Krikorian and Wallace	149
1700 ± 21	1754 ± 28	Langer <i>et al.</i>	145

THORIUM-URANIUM DICARBIDE [(Th_{0.9}U_{0.1})C₂]Melting Point: 2900 K

This value is a calculated molar average. The phase diagram given in Fig. 24, page 101, of Ref. 3 indicates an incorrect melting point for ThC₂. We assumed no minimum in the melting diagram (as stated on page 102 of the report) and used a molar average.

Enthalpy, H_(MP) - H₍₂₉₈₎: 222 kJ/mol

This value is a calculated molar average. No data exist.

Heat of Fusion, ΔH_m: 67 kJ/mol

This value was calculated assuming that the heat of fusion = nR, where n is the number of gram atoms in the compound. No experimental data exist.

Heat Capacity, C_{P(298)}: 57.3 J/K mol

This is a calculated molar average. No experimental data exist.

Heat Capacity, C_{P(MP)}^(s): 87.9 J/K·mol

This is a calculated molar average. No experimental data exist.

Thermal Conductivity, K₍₂₉₈₎: 18.8 W/m·K

This value was extrapolated from tabulated experimental data in Ref. 3. Measurements have been made from 473 to 1223 K by Griesenauer *et al.*¹²³

Density, ρ₍₂₉₈₎^(s): 9.8 x 10³ kg/m³

This value is a molar average. Apparently no experimental data exist.

Density, ρ_(MP)^(s): 9.1 x 10³ kg/m³

This value was calculated using the coefficients of thermal expansion given by Peterson and Curtis in Ref. 3.

Volumetric Thermal Expansion Coefficient, α_(298-MP)^(s): 2.7 x 10⁻⁵ K⁻¹

This value is based on tabulated values³ of linear thermal expansion coefficients measured by Cook to 1300 K.¹⁴⁶

URANIUM DICARBIDE (UC₂)

Melting Point: 2780 K

This is the melting point recommended by Fee and Johnson.¹³⁴

Enthalpy, $H_{(MP)} - H_{(298)}$: 256.0 kJ/mol

This value is recommended by Storms and Ackermann¹²⁷ based on experiments to 1600 K. The maximum temperature of UC₂ experimental data is 2500 K. However, these data are uncertain owing to composition changes during the experiment. UC₂ enthalpy data are probably reliable to 1600 K.

Heat of Fusion, ΔH_m : 67 kJ/mol

This value was calculated assuming the heat of fusion = nR, where n is the number of gram atoms in the compound.

Heat Capacity, $C_{P(298)}$: 60.7 J/K·mol

This is the recommended value by the IAEA Panel.¹²⁷

Heat Capacity, $C_{P(MP)}^{(s)}$: 123.0 J/K·mol

This value is recommended by Storms and Ackermann¹²⁷ based on experiments to 1600 K. The maximum temperature of experimental data is 2500 K. However, these data are uncertain due to composition changes during the experiment. UC₂ enthalpy and heat capacity data are probably reliable to 1600 K.

Density, $\rho_{(298)}^{(s)}$: 1.17×10^4 kg/m³

This value was calculated from the lattice parameters¹⁵⁰ for UC₂. No density measurements exist.

Density, $\rho_{(MP)}^{(s)}$: 1.06 kg/m³

This value was calculated by us using the thermal expansion coefficients given by Peterson and Curtis in Ref. 3.

Volumetric Thermal Expansion Coefficient, $\bar{\alpha}_{(298-MP)}^{(s)}$: 4.0×10^{-5} K⁻¹

This value is from tabulated values³ of linear thermal expansion coefficients measured by Cook to 1300 K.¹⁴⁶

APPENDIX

To facilitate the comparison of properties of thorium and uranium systems, plots of some properties are included here. Figure 1 plots the vapor pressure of thorium and uranium metals as a function of temperature. Figures 2 to 4, respectively, show the heat capacities, enthalpies, and vapor pressures of both ThO_2 and UO_2 as a function of temperature. Figure 5 is a plot of pressure *vs.* enthalpy for ThO_2 and UO_2 . On each curve, the highest temperature at which experimental data exist is indicated by an arrow pointing to that temperature.

Fig. 1. Vapor Pressure vs. Temperature for Thorium and Uranium

Fig. 2. Heat Capacity vs. Temperature for ThO_2 and UO_2

Fig. 3. Enthalpy vs. Temperature for ThO_2 and UO_2

Fig. 4. Vapor Pressure vs. Temperature for ThO₂ and UO₂

Fig. 5. Pressure vs. Enthalpy for ThO₂ and UO₂

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