

Estimating Solid–Liquid Phase Change Enthalpies and Entropies

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A group additivity method based on molecular structure is described that can be used to estimate solid–liquid total phase change entropy ($\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$) and enthalpy ($\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$) of organic molecules. The estimation of these phase changes is described and numerous examples are provided to guide the user in evaluating these properties for a broad range of organic structures. A total of 1858 compounds were used in deriving the group values and these values are tested on a database of 260 additional compounds. The absolute average and relative errors between experimental and calculated values for these 1858 compounds are $9.9 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ and $3.52 \text{ kJ}\cdot\text{mol}^{-1}$, and 0.154 and 0.17 for $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$, respectively. For the 260 test compounds, standard deviations of $\pm 13.0 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ ($\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$) and $\pm 4.88 \text{ kJ}\cdot\text{mol}^{-1}$ ($\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$) between experimental and calculated values were obtained. Estimations are provided for both databases. Fusion enthalpies for some additional compounds not included in the statistics are also included in the tabulation. © 1999 American Institute of Physics and American Chemical Society. [S0047-2689(99)00106-3]

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1. Introduction

1.1. Fusion Enthalpies

Fusion enthalpy is an important physical property of the solid state. The magnitude of the fusion enthalpy influences solute solubility in both an absolute sense and in its temperature dependence. This property plays an important factor in determining molecular packing in crystals and can be useful in correcting thermochemical data to a standard state when combined with other thermodynamic properties.

The discrepancy in numbers between the many new organic solids prepared and the few thermochemical measurements reported annually has encouraged the development of empirical relationships that can be used to estimate properties such as fusion enthalpy. We have found that techniques for estimating fusion enthalpies can play several useful roles.¹⁻³ Perhaps most importantly, they provide a numerical value that can be used in cases when there are no experimental data. Estimations are also useful in selecting the most probable experimental value in cases where two or more values are in significant disagreement. Given the choice between an estimated or experimental value, selection of the experimental value is clearly preferable. However, large discrepancies between estimated and calculated values can also identify systems exhibiting dynamic or associative properties. Some molecular systems exhibit phase transitions that occur in the solid state that are related to the onset of mo-

lecular motion. Others, such as liquid crystals exhibit nonisotropic molecular motion in the liquid phase.⁴ Both have associated with these phenomena, additional phase transitions that attenuate the enthalpy and entropy associated with fusion. A large positive discrepancy in the difference between estimated and experimentally measured fusion enthalpy is a good indication of this behavior.

1.2. Fusion Entropies

Very few general techniques have been developed for directly estimating fusion enthalpies, in part, as a consequence of the complex phase behavior exhibited by some compounds. Fusion enthalpies have been most frequently calculated from fusion entropies and the experimental melting temperature of the solid T_{fus} . One of the earliest estimation techniques is the use of Walden's Rule.⁵ The application of Walden's Rule provides a remarkably good approximation of $\Delta_{\text{fus}}H_m$, if one considers that the estimation is independent of molecular structure and based on only two parameters. Recent modifications of this rule have also been reported.^{6,7} Walden's Rule:

$$\begin{aligned} \Delta_{\text{fus}}H_m(T_{\text{fus}})/T_{\text{fus}} &\approx 13 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1} \\ &= 54.4 \text{ J mol}^{-1}\text{K}^{-1}. \end{aligned} \quad (1)$$

A general method for estimating fusion entropies based on the principles of group additivity has been reported recently.⁸⁻¹⁰ This method has been developed from the assumption that unlike fusion enthalpy and entropy, the total phase change entropy associated in going from a rigid solid at 0 K to an isotropic liquid at the melting point, T_{fus} , is a group property and that this property can be estimated by standard group additivity techniques. The total phase change entropy has been defined as the sum of the entropy associated with all the phase changes occurring in the condensed phase prior to and including melting. The assumption that the total phase change entropy is a more reliable group property than fusion entropy is readily apparent from an examination of these two properties as a function of the number of methylene groups for the *n*-alkanes. This is illustrated in Figs. 1 and 2. Many alkanes have additional phase transitions with significant entropy components that influence the magnitude of the fusion entropy. This leads to the nonlinear behavior illustrated in Fig. 1. When these components are added together, the total phase change entropy shows a much better linear correlation. Some odd-even alternation as a function of the number of carbon atoms is evident similar to what is observed in the melting points of these compounds

2. Estimation of Total Phase Change Entropy and Enthalpy

2.1. Derivation of Group Values

Initial group values for a methyl and methylene group were derived from the intercept (one half the intercept) and

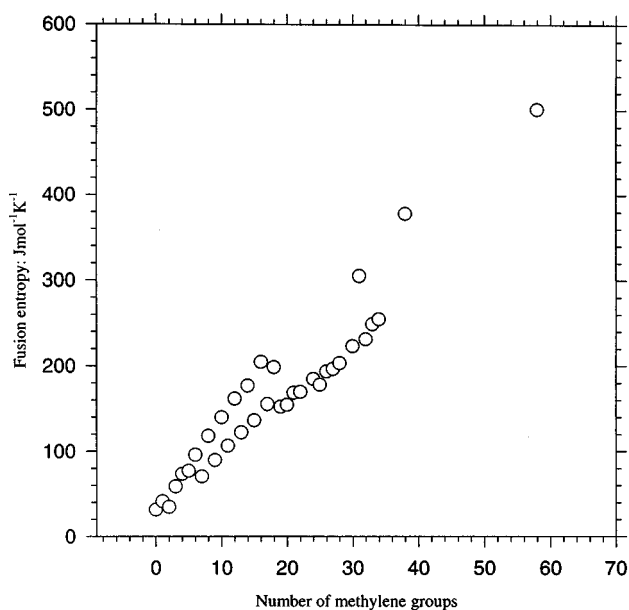


FIG. 1. Fusion entropy of the *n*-alkanes as a function of the number of methylene groups.

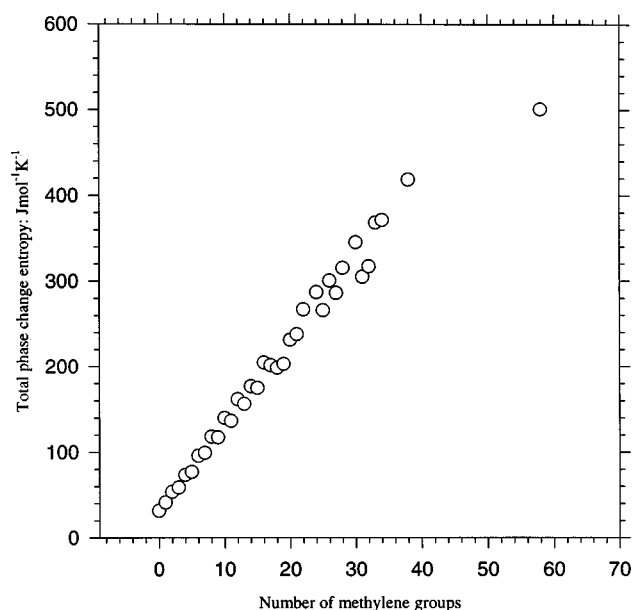


FIG. 2. Total phase change entropies of the *n*-alkanes as a function of the number of methylene groups.

slope of the line of Fig. 2, respectively. Group values for carbon in other common environments were initially derived from experimental data of compounds with appropriate structures using these two group values. Subsequent refinements were possible as additional experimental data became available. Once values were assigned for most carbon groups, these values were allowed to vary until the value of the function:

$$\sum_{i=1}^n [\Delta_0^{T_{\text{fus}}} S(\text{expt}) - \Delta_0^{T_{\text{fus}}} S(\text{calcd})]^2$$

did not change significantly upon successive iterations. Group values for the functional groups were derived in a similar fashion. Using group values for carbon established from the hydrocarbons, values for the functional groups in Tables 1 and 2 were derived. Once initial values for these groups were established, a similar least squares minimization of all the values were performed.

The total phase change entropy, $\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$, in most cases provides a good estimate of the entropy of fusion, $\Delta_{\text{fus}} S_m(T_{\text{fus}})$. If there are no additional solid phase transitions then $\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ becomes numerically equal to $\Delta_{\text{fus}} S_m(T_{\text{fus}})$. From the experimental melting point and $\Delta_{\text{fus}} S_m(T_{\text{fus}})$, it is possible to approximate the total phase change enthalpy, $\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$. Similarly, if there are no additional phase transitions then the total phase change enthalpy, $\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$, becomes numerically equivalent to the fusion enthalpy, $\Delta_{\text{fus}} H_m(T_{\text{fus}})$.

A listing of the group parameters that can be used to estimate these phase change properties is presented in Tables 1 and 2. The group values in these tables have been updated from previous versions by the inclusion of new experimental data in the parameterizations.^{8,9} Before describing the appli-

cation of these parameters in the estimation of $\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$, the conventions used to describe these group values need to be defined. Primary, secondary, tertiary, and quaternary centers, as found on atoms of carbon, silicon, and their congeners, are defined solely on the basis of the number of hydrogens attached to the central atom, 3, 2, 1, 0, respectively. It should be noted that the experimental melting point along with an estimated value of $\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ is necessary to estimate the fusion enthalpy of a compound. In addition, compounds whose liquid phase is not isotropic at the melting point are not modeled properly by these estimations. Those compounds forming liquid crystal or cholesteric phases as well amphiphilic compounds are currently overestimated by these parameters. A large discrepancy between the estimated total phase change enthalpy and experimental fusion enthalpy is a good indication of undetected solid–solid phase transitions or anisotropic liquid behavior.

The parameters used for estimating $\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ of hydrocarbons and the hydrocarbon portions of more complex molecules are listed in Table 1. The group value, G_i , associated with a molecular fragment is identified in the third column of the table. The group coefficients, C_i , are listed in column 4 of the table. These group coefficients are used to modify G_i whenever a functional group is attached to the carbon in question. Functional groups are defined in Table 2. Group values reported in parenthesis are based on only a limited database (arbitrarily chosen as less than seven entries) and should be considered as tentative assignments. All values of C_i and C_k that are not specifically defined in Tables 1 and 2 are to be assumed equal to 1.0. The group coefficient for a methylene group in Table 1, C_{CH_2} , is applied differently from the rest and its application is discussed below. Introduction of this coefficient is new and differentiates this pro-

to col from earlier versions. The application of this group coefficient as well as the entire protocol is illustrated in the examples given in Tables 3 and 4.

3. Estimations of Hydrocarbons

3.1. Acyclic and Aromatic Hydrocarbons

Estimation of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ for acyclic and aromatic hydrocarbons (*ah*) can be achieved by summing the group values consistent with the structure of the molecule as illustrated by the following equation:

$$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(ah) = \sum_i n_i G_i + n_{\text{CH}_2} C_{\text{CH}_2} G_{\text{CH}_2};$$

$$C_{\text{CH}_2} = 1.31 \text{ when } n_{\text{CH}_2} \geq \sum n_i;$$

$$i \neq \text{CH}_2 \text{ otherwise } C_{\text{CH}_2} = 1. \quad (2)$$

The group coefficient for a methylene group C_{CH_2} is used whenever the total number of consecutive methylene groups in a molecule n_{CH_2} equals or exceeds the sum of the other remaining groups $\sum n_i$. This applies to both hydrocarbons and all derivatives. In oligomers, and polymers, the decision as to whether to include this group coefficient should be based on the structure of the repeating unit. Some examples illustrating the use of both the groups in Table 1(a) and Eq. (2) are given in Table 3 and additional discussion regarding the use of C_{CH_2} is provided in the discussion that pertains to polymers below. Entries for each estimation in Table 3 include the melting point T_{fus} and all transition temperatures T_i for which there is a substantial enthalpy change. The estimated and experimental (in parentheses) phase change entropies follow. Similarly, the total phase change enthalpy calculated as the product of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and T_{fus} is followed by the experimental total phase change enthalpy (or fusion enthalpy). Finally, details in estimating $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ for each compound are included as the last entry for each compound.

3.1.1. Styrene

The estimation of the fusion entropy of styrene is an example of an estimation of a typical aromatic hydrocarbon. Identification of the appropriate groups in Table 1(a) results in an entropy of fusion of $52.5 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ and together with the experimental melting point, an enthalpy of fusion of $12.6 \text{ kJ}\cdot\text{mol}^{-1}$ is estimated. This can be compared to the experimental value of $11.0 \text{ kJ}\cdot\text{mol}^{-1}$. It should be pointed out that the group values for aromatic molecules are purely additive while the group values for other cyclic sp^2 atoms, summarized in Table 1(b), are treated as corrections to the ring equation. This will be discussed in more detail below.

3.1.2. 1-Heptene

The fusion entropy of 1-heptene is obtained in a similar fashion. In this case, the number of consecutive methylene groups in the molecule exceeds the sum of the remaining

terms in the estimation and this necessitates the use of the group coefficient C_{CH_2} of 1.31. For a molecule such as 3-heptene (estimation not shown), the group coefficient of 1.31 would not be applied. For a molecule such as 3-decene (also not shown), the group coefficient of 1.31 would be applied only to the five consecutive methylene groups. The remaining methylene group at carbon 2 would be treated normally ($C_{\text{CH}_2} = 1.0$) and would not be counted in $\sum n_i$.

3.1.3. Perylene

Estimation of the phase change entropy of perylene provides an example of a molecule containing both peripheral and internal quaternary sp^2 carbon atoms adjacent to an sp^2 atom. The carbon atoms in graphite are another example of internal quaternary sp^2 carbon atoms. In the application of these group values to obtain the phase change properties of other aromatic molecules, it is important to remember that the aromatic portion of a molecule is defined in these estimations as molecules containing only benzenoid carbons and the corresponding nitrogen heterocycles. While a molecule like 1,2-benzacenaphthene (fluoranthene) would be considered aromatic, the five membered ring in acenaphthylene, according to this definition is not. Estimation of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ for acenaphthylene will be illustrated below.

3.2. Nonaromatic Cyclic and Polycyclic Hydrocarbons

The protocol established for estimating $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ of unsubstituted cyclic hydrocarbons uses Eq. (3) to evaluate this term for the parent cycloalkane, $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{ring})$. For substituted and polycyclic cycloalkanes,

$$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{ring}) = [33.4] + [3.7][n - 3];$$

$$n = \text{number of ring atoms}, \quad (3)$$

$$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{ring}) = [33.4]N + [3.7][R - 3N];$$

$$R = \text{total number of ring atoms}; N = \text{number of rings}, \quad (4)$$

the results of Eqs. (3) or (4), respectively, are then corrected for the presence of substitution and hybridization patterns in the ring that differ from the standard cyclic secondary sp^3 pattern found in the parent monocyclic alkanes, $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{corr})$. These correction terms can be found in Table 1(b). Once these corrections are included in the estimation, any additional acyclic groups present as substituents on the ring are added to the results of Eqs. (3) or (4) and $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{corr})$. These additional acyclic and/or aromatic terms $[\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(ah)]$ are added according to the protocol discussed above in the use of Eq. (2). The following ex-

amples of Table 3 illustrate the use of Eq. (3) and (4) according to Eq. (5) to estimate the total phase change entropy of cyclic molecules $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{total})$:

$$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{total}) = \Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{ring}) + \Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{corr}) + \Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{aah}). \quad (5)$$

3.2.1. 10,10,13,13-Tetramethyl-1,5-cyclohexadecadiyne

The estimation of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ for 10,10,13,13-tetramethyl-1,5-cyclohexadecadiyne illustrates the use of Eq. (5) for a monocyclic alkyne. Once the hexadecane ring is estimated ($[33.4] + 13[3.7]$), correcting for the presence of two cyclic quaternary sp^3 carbon atoms ($2[-34.6]$), four cyclic sp carbon atoms ($4[-4.7]$) and four methyl groups ($4[17.6]$) completes this estimation.

3.2.2. Bullvalene

Bullvalene, a tricyclic hydrocarbon, provides an example of the use of Eqs. (4) and (5). The minimum number of bonds that need to be broken to form a completely acyclic molecule is used to determine the number of rings. In this case it is three. Application of Eq. (4) to bullvalene [$3[33.4] + 3.7[10-9]$] provides $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{ring})$. Addition of the contributions of the four cyclic tertiary sp^3 carbons and the six tertiary sp^2 carbons to the results of Eq. (4), $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{corr})$, completes the estimation.

3.2.3. Acenaphthylene

Estimation of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ for acenaphthylene completes this section on cyclic hydrocarbons. Molecules that contain rings fused to aromatic rings but are not completely aromatic, according to the definition provided above, are estimated by first calculating $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{ring})$ for the contributions of the nonaromatic ring according to Eqs. (3) or (4). The atoms of the nonaromatic ring should be selected on the basis of the smallest number of ring atoms that account for all the nonaromatic carbons. This is then followed by addition of the adjustments for the nonsecondary sp^3 ring carbons, the contributions of the remaining aromatic groups and any other substituents that may be present. In acenaphthylene, the contribution of the five membered ring $\{\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{ring}): [33.4] + 2[3.7]\}$ is first adjusted for each nonsecondary sp^3 carbon atom in the ring $\{\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{corr}): +2[-1.6] + 3[-12.3]\}$, and then the remainder of the aromatic portion of the molecule is added $\{\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{aah}): [-7.5] + 6[7.4]\}$. In a molecule such as $[2,2]\text{-meta-cyclophane}$ (estimation not shown), the acyclic ring the chosen to contain the fewest ring atoms, ten carbons in this instance. The six aromatic ring atoms that make up a portion of the ten membered ring are considered as cyclic sp^2 carbon atoms (four quaternary sp^2 and two tertiary sp^2

carbons). Addition of the contributions of the six remaining aromatic tertiary carbon atoms not included in the aliphatic ring completes this estimation.

4. Estimations of Hydrocarbon Derivatives

Estimations involving derivatives of hydrocarbons are performed in a fashion similar to hydrocarbons. The estimation consists of three parts: the contribution of the hydrocarbon component, that of the carbon(s) bearing the functional group(s), $\sum_i n_i C_i G_i$, and the contribution of the functional group(s) $\sum_k n_k C_j G_k$. The symbols n_i , n_k refer to the number of groups of type i and k . Acyclic and cyclic compounds are treated separately as before. For acyclic and aromatic molecules, the hydrocarbon portion is estimated using Eq. (2); cyclic or polycyclic molecules are estimated using Eqs. (3) and (4), respectively. Similarly, the contribution of the carbon(s) bearing the functional group(s) is evaluated from Tables 1 (a) or 1(b) modified by the appropriate group coefficient C_i as will be illustrated below. The group values of the functional groups G_k are listed in Tables 2(a) and 2(b). The corresponding group coefficient C_j is equal to one for all functional groups except those identified otherwise in Table 2(a). Selection of the appropriate value of C_j from Table 2(a) is based on the total number of functional groups and is discussed below. Functional groups that make up a portion of a ring are listed in Table 2(b). The use of these values in estimations will be illustrated separately. Equations (6) and (7) summarize the protocol developed to estimate $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{total})$ for acyclic and aromatic derivatives and for cyclic and polycyclic hydrocarbon derivatives, respectively,

$$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{total}) = \Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{aah}) + \sum_i n_i C_i G_i + \sum_k n_k C_j G_k, \quad (6)$$

$$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{total}) = \Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{ring}) + \Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{corr}) + \sum_i n_i C_i G_i + \sum_k n_k C_j G_k, \quad (7)$$

where

$$C_j = \sum_k n_k.$$

In view of the large number of group values listed in Tables 2(a) and 2(b), selection of the appropriate functional group(s) is particularly important. Four functional groups in Table 2(a), chlorine, the hydroxyl and carboxyl group, and tri-substituted amides are dependent on the total substitution pattern in the molecule. Coefficients for these four groups C_j are available for molecules containing up to six functional groups. Selection of the appropriate value of C_j for one of these four functional groups is based on the total number of functional groups in the molecule. Estimations of the fusion entropy of polymers suggests that the group coefficient for C_6 in Table 2(b), is adequate for molecules containing more than a total of six functional groups.¹⁹

4.1. Acyclic and Aromatic Hydrocarbon Derivatives

The estimations for decachlorobiphenyl, N-acetyl-L-alanine amide, 2,2,2-trifluoroacetonitrile, and isoquinoline, shown in Table 4(a), illustrate the estimations of substituted aromatic and acyclic hydrocarbon derivatives.

4.1.1. Decachlorobiphenyl

Decachlorobiphenyl is an example of an estimation of a polysubstituted aromatic molecule. Selection of the value for a quaternary aromatic sp^2 carbon from Table 1(a) depends on the nature of the functional group attached to carbon. If the functional group at the point of attachment is sp^2 hybridized or contains nonbonding electrons, the value for a "peripheral aromatic sp^2 carbon adjacent to an sp^2 atom" is selected. Otherwise a "peripheral aromatic sp^2 carbon adjacent to an sp^3 atom" is used. The remainder of the estimation follows the guidelines outlined above with the exception that chlorine is one of the four functional groups whose group coefficient C_j depends on the degree of substitution (C_6 is used in this example).

4.1.2. N-acetyl-L-alanine amide

The estimation of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ for N-acetyl-L-alanine amide follows directly from Eq. (6). The molecule contains both a primary and secondary amide linkage. The asymmetric center is a tertiary carbon that contains two functional groups attached to it and as such its contribution is attenuated by the group coefficient for a tertiary carbon. Addition of the contributions of the two methyl groups completes the estimation.

4.1.3. Trifluoroacetonitrile

The estimation of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ for trifluoroacetonitrile illustrates an example of a molecule containing fluorine. The group value for a fluorine on a trifluoromethyl group in Table 2(a) is given per fluorine atom. The contribution of the quaternary carbon atom when attached to functional groups is attenuated by the group coefficient C_i . Inclusion of the group value for a thiol completes this estimation. When fluorine is combined with the functional groups listed in Table 2(b), the group coefficient chosen should be based on the presence of fluorine as a single functional group, regardless of the number of fluorine atoms present. For example, a molecule such as trifluoromethanol would be considered to contain two functional groups.

4.1.4. Isoquinoline

The estimation of isoquinoline illustrates an example of another aromatic molecule. The only exception in this case is the need to substitute the group value for a heterocyclic aromatic amine. Otherwise the same protocol is followed as in the estimation of naphthalene (not shown).

4.2. Cyclic and Polycyclic Hydrocarbon Derivatives

The protocol for estimating the total phase change properties of cyclic and polycyclic molecules also follows from the procedure described above for the corresponding cyclic hydrocarbons. In cyclic molecules, the substituent or functional group may be attached to the ring or it may be part of the ring. If the functional group is part of the ring, the group values listed in Table 2(b) are to be used. The procedure first involves estimating $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ for the corresponding hydrocarbon ring, then correcting for the heterocyclic component(s), and if necessary, correcting the ring carbons attached to the cyclic functional group by the appropriate group coefficients. This is illustrated in Table 4(b) by the following examples.

4.2.1. 2-Chlorodibenzodioxin

The dioxane ring of 2-chlorodibenzodioxin is treated as being a derivative of cyclohexane. According to Eq. (7), the ring equation is first used to estimate the contributions of the cyclohexane ring. This ring contains two cyclic ether oxygens and four quaternary cyclic sp^2 carbon atoms and must be modified accordingly. The remaining eight carbon atoms are treated as aromatic carbons and values appropriate to their substitution pattern are chosen. The addition of the contribution of the chlorine completes the estimation.

4.2.2. 6,8,9-Trimethyladenine

6,8,9-Trimethyladenine is estimated in a similar fashion. The ring equation [Eq. (3)] is used first to generate the contribution of the five membered heterocyclic ring. In this instance the ring has been modified by the addition of a cyclic sp^2 hybridized nitrogen atom and a nitrogen which comprises part of a cyclic tertiary amine. Both ring substitutions require appropriate corrections. The hybridization and substitution of the remaining three cyclic carbon atoms of the five membered ring have likewise been changed from the pattern found in cyclopentane and appropriate changes must also be included in $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(\text{corr})$. The remaining four ring atoms comprise a portion of an aromatic ring; their contributions can be added directly. The two nitrogen atoms make up a portion of the heterocyclic aromatic ring along with a quaternary and tertiary aromatic sp^2 carbon atom. The quaternary aromatic sp^2 carbon atom is attached to an exocyclic nitrogen atom with a lone pair of electrons and consequently, the quaternary aromatic carbon is treated as being adjacent to an sp^2 center. The contributions of the tertiary aromatic sp^2 carbon atom, the methyl groups, and the acyclic secondary amine complete the estimation.

4.2.3. Lenacil

Estimations of Lenacil (3-cyclohexyl-6,7-dihydro-1H-cyclopentapyrimidine-2,4-(3H,5H)-dione) require some thought in properly identifying the functional groups in the molecule. The functional group that makes up a portion of the pyrimidine-2,4-dione ring in this molecule cannot be

found directly in Table 2(b). It must therefore be simplified and this simplification can be accommodated in various ways. The ring can be considered to be a combination of either an adjacent cyclic imide ($-\text{CONRCO}-$) and cyclic amide nitrogen ($-\text{NH}-$), a cyclic urea ($-\text{NRCONH}-$) and amide carbonyl ($-\text{CO}-$), or a cyclic secondary and tertiary amide. An examination of the available groups in Table 2(b) will reveal that although group values for cyclic imides are available ($-\text{NRCONH}-$, $-\text{NRCONR}-$), there is no appropriate group available for an N-substituted cyclic nitrogen of an amide. Similarly, group values for a cyclic urea and amide carbonyl are not available. The most appropriate group values that are available are for cyclic amides. Once the appropriate group is identified, the procedure follows the same protocol as established for other polycyclic molecules.

4.2.4. Cortisone

The estimation of the fusion enthalpy of cortisone illustrates an example of an estimation of a complex polycyclic compound. This tetracyclic 17 atom ring system contains three cyclic quaternary centers ($3[-34.6]$), three cyclic tertiary sp^3 centers, ($3[-14.7]$), a cyclic tertiary sp^2 center which is attached to a functional group [1.92][-1.6], a quaternary sp^2 center ($[-12.3]$) as well as two cyclic carbonyl group ($2[-1.4]$). Addition of these modifications to the ring equation ($4[33.4]+5[3.7]$) estimates the contributions of the ring. Addition of the contributions of the substituents which include three hydroxyls ($(3)(12.1)[1.7]$), two methyls ($2[17.6]$), a methylene ($[7.1]$), and a carbonyl group of an acyclic ketone ($[4.6]$) completes the estimation. The molecule contains five functional groups, hence C_5 for a hydroxyl group is used.

4.3. Polymers

In addition to the estimation of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ of small molecules, the parameters of Tables 1 and 2 can be used to predict $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (when the experimental melting point is known) of crystalline oligomers and linear polymers. Since the parameters in Tables 1 and 2 differ slightly from those reported previously,¹⁹ the predictions of Eqs. (2)–(6) likewise produce slightly different results. However a similar overall correlation (slightly improved) between experimental and calculated results is obtained using the updated parameters. The protocol used to evaluate $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ of polymers is exactly the same as outlined above. In this instance, the entropic value is calculated on the basis of the structure of the repeat unit of the polymer. Best correlations are obtained when the group coefficient C_k chosen is based on the number of functional groups present on the repeat unit and on the two nearest neighbors. The polymer $(\text{CH}_2\text{O})_n$, is treated as an infinite chain with $n_0 = n_{\text{CH}_2}$. For a molecule such as $\text{CH}_3\text{O}(\text{CH}_2\text{CH}_2\text{O})_n\text{CH}_3$, the number of methylene groups in the repeat unit exceeds the number of oxygens and therefore the group coefficient for a methylene group should be used. As n becomes smaller, a point will be reached when the molecule no longer represents an oligomer. In this in-

stance the group coefficient for a methylene group should be dropped. This should occur when n becomes less than the number of other groups that make up the remainder of the molecule. In the case just described, this would occur when n becomes less than three.

The column entries in Tables 6 and 7 are identical (these data were not used in generating the group values of Tables 1 and 2) and are described below. Calculated and experimental values of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ for a series of linear polymers are provided in Table 6.

5. The Group Coefficient in Cycloalkyl Derivatives

The protocol in determining whether to use the group coefficient C_{CH_2} depends on whether the number of consecutive methylene groups exceeds the sum of the remaining groups excluding other methylene groups in the count. In an estimation of a cyclic derivative, the contribution of the ring is determined by Eq. (3) or (4) along with other terms necessary to correct for substitution and hybridization changes. This will vary depending on the nature of the ring and its substitution patterns. Fewer terms are necessary to estimate the total phase change entropy of ethylcyclohexane than ethylcyclohexadiene, even though in principle, both contain the same number of groups. To avoid any ambiguity in determining when to use this group coefficient, the number of groups associated with a ring structure should be determined by the size of the ring and the number of substituents or functional groups attached to the ring. For example, a molecule such as 2,5-di-*n*-undecyloxy-1,4-benzoquinone, contains 10 adjacent methylene groups. These methylene groups should be compared to the total number of other groups on the molecule. This includes two carbonyls, two methyl groups, two ether oxygens, and four sp^2 hybridized carbon atoms, adding up to a total of 10. Since these two numbers are equal, the group coefficient should be applied to both undecyl groups.

6. Polymorphism

In some cases, particularly with some pharmaceuticals, different fusion enthalpies and melting points have been reported for the same material. For example, fusion enthalpies of $18\,284$ (428.2 K)²⁰ and $23\,810\text{ J mol}^{-1}$ (430.3 K)²¹ have been reported for codeine. While one of these values may be in error, the two values may represent accurate physical properties of different crystalline modifications of codeine. The value estimated by the group additivity approach described above generally gives total phase change entropies and enthalpies associated with the most stable modification at the melting point. A recent review article summarizes pharmaceuticals known to exhibit polymorphism.²²

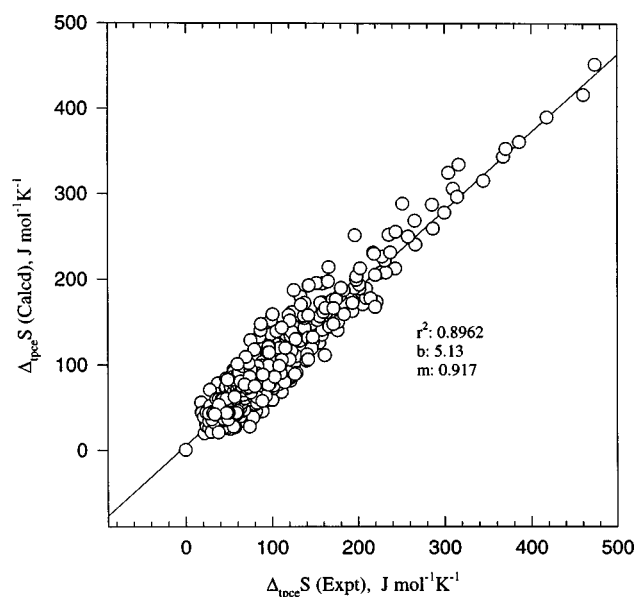


FIG. 3. A comparison of calculated and experimental $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ of 1858 database compounds.

7. Statistics of the Correlation

7.1. Database Compounds

The group values included in Tables 1 and 2 were generated from the fusion entropies of a total of 1858 compounds. Melting and transition temperatures (column 1), experimental enthalpies associated with all solid–solid and solid–liquid phase changes (ΔH_{pce} , column 2), the corresponding phase change entropies (ΔS_{pce} , column 3), the total experimental phase change entropy (column 4) and enthalpy (columns 6), and the corresponding values estimated from the group values of Tables 1 and 4 (columns 5 and 7) for each of these compounds are given in Table 5. A summary of each calculation is also included in the form of the alphanumeric terms

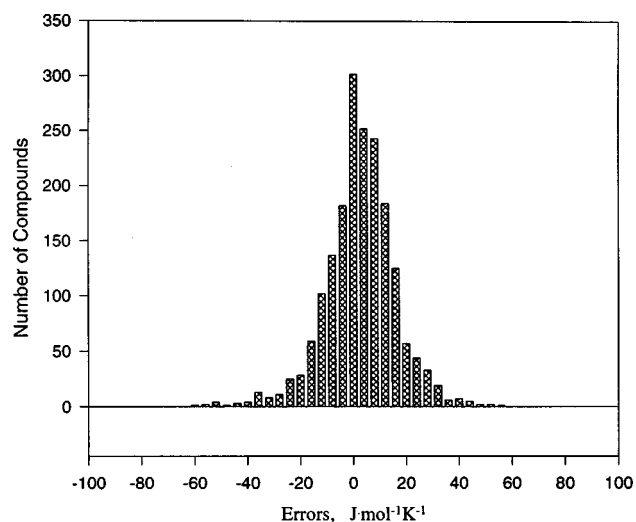


FIG. 4. A histogram illustrating the distribution of errors in estimating $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ of the database compounds.

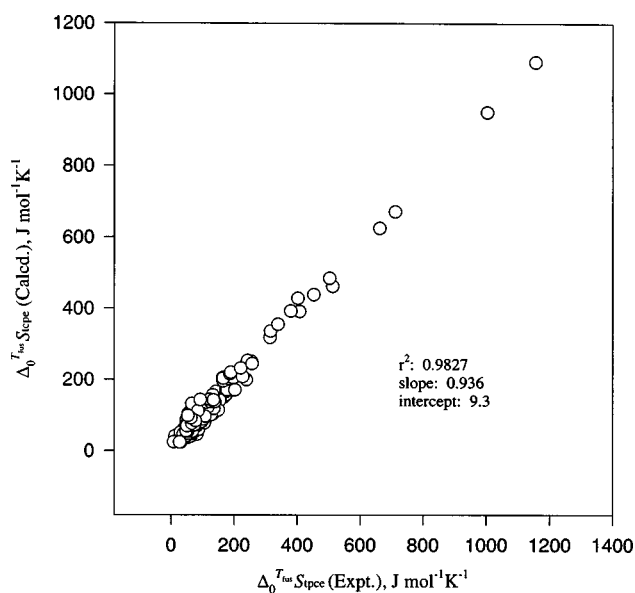


FIG. 5. A comparison of calculated and experimental $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ of 260 test compounds.

used in each calculation. These alphanumeric terms are defined in Tables 1 and 2 for each group (in parenthesis). Table 5 also includes a number of compounds that were not included in deriving either the statistics or the group values. Reasons for this are noted in the table. An asterisk following the molecular formula in the table identifies these materials. Experimental and calculated total phase change entropies for the database are compared in Fig. 3. The correlation was characterized by the slope m , intercept b , and correlation coefficient (r^2) given in the figure. A histogram of the errors associated with this correlation is shown in Fig. 4. The absolute average and relative errors between experimental and

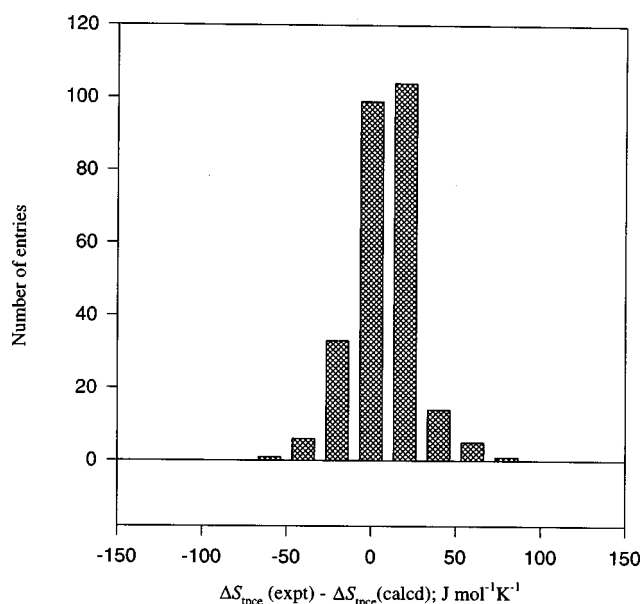


FIG. 6. A histogram illustrating the distribution of errors in estimating $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ of 260 test compounds.

calculated $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ values for these 1858 compounds are $9.9 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ and $3.52 \text{ kJ}\cdot\text{mol}^{-1}$, and 0.154 and 0.17, respectively. The standard deviations between experimental and calculated values for $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ are $\pm 13.0 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ and $\pm 4.88 \text{ kJ}\cdot\text{mol}^{-1}$, respectively. An additional 60 compounds exhibited errors exceeding 3 s.d. and were excluded from the correlations and from Figs. 3 and 4. These compounds are included in Tables 5 and 7.

7.2. Test Compounds

In addition to the 1858 compounds that make up the database, an additional 260 compounds have been used as test materials to provide an unbiased evaluation of the reliability of the group values given in Tables 1 and 2. These fusion enthalpies include compounds obtained from more recent

searches of the literature and are reported in Table 7. The data included in Table 7 are in the same format as the data in Table 5. The correlation between experimental and calculated values for the test compounds is shown in Fig. 5. The standard deviations between experimental and calculated values for $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ were $\pm 18.4 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ and $\pm 7.2 \text{ kJ}\cdot\text{mol}^{-1}$, respectively. The absolute average and relative errors between experimental and calculated $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ values for these 260 compounds were $13.9 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ and $5.28 \text{ kJ}\cdot\text{mol}^{-1}$, and 0.181 and 0.194, respectively. In addition to these 260 compounds, some recently acquired data are also included in Table 7. As before, compounds not included in the correlations are identified by an asterisk following their molecular formula (see Tables 5, 6, and 7). References to Tables 5, 6, and 7 are listed in Table 8.

TABLE 1. (a) Contributions of the hydrocarbon portion of acyclic and aromatic molecules

Acyclic and aromatic carbon groups	Group value ^a G_i ($\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$)	Group coefficients ^a C_i
primary sp^3	CH_3- 17.6 (A1)	
secondary sp^3	$>\text{CH}_2$ 7.1 (A2)	1.31 ^b (B2)
tertiary sp^3	$-\text{CH}<$ -16.4 (A3)	0.60 (B3)
quaternary sp^3	$>\text{C}<$ -34.8 (A4)	0.66 (B4)
secondary sp^2	$=\text{CH}_2$ 17.3 (A5)	
tertiary sp^2	$=\text{CH}-$ 5.3 (A6)	0.75 (B6)
quaternary sp^2	$=\text{C}(\text{R})-$ -10.7 (A7)	
tertiary sp	$\text{H}-\text{C}\equiv$ 14.9 (A8)	
quaternary sp	$-\text{C}\equiv$ -2.8 (A9)	
aromatic tertiary sp^2	$=\text{C}_a\text{H}-$ 7.4 (A10)	
quaternary aromatic sp^2 carbon adjacent to an sp^3 atom	$=\text{C}_a(\text{R})-$ -9.6 (A11)	
peripheral quaternary aromatic sp^2 carbon adjacent to an sp^2 atom	$=\text{C}_a(\text{R})-$ -7.5 (A12)	
internal quaternary aromatic sp^2 carbon adjacent to an sp^2 atom	$=\text{C}_a(\text{R})-$ -0.7 (A13)	

^aThe alphanumeric terms, A1, A2, B2, ... are a device used to identify each group value in the estimations provided in Tables 7, 8, and 9.

^bThe group coefficient of 1.31 for C_{CH_2} is applied only when the number of consecutive methylene groups equals or exceeds the sum of the remaining groups; see Eq. 2 in text.

TABLE 1. (b) Contributions of the cyclic hydrocarbon portions of the molecule

Contributions of cyclic carbons	Group value (G_i) ($\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$)	Group coefficient C_i
Ring equations for nonaromatic cyclic compounds		
$\Delta S_{\text{ring}} = [33.4(A14)] + [3.7(A15)][n - 3]$; $n = \text{number of ring atoms}$		
Ring equation for nonaromatic polycyclic compounds		
$\Delta S_{\text{ring}} = [33.4(A14)]N + [3.7(A15)][R - 3N]$; $R = \text{total number of ring atoms}$; $N = \text{number of rings}$		
cyclic tertiary sp^3	$>\text{C}_c\text{H}(\text{R})$ -14.7 (A16)	
cyclic quaternary sp^3	$>\text{C}_c(\text{R})_2$ -34.6 (A17)	
cyclic tertiary sp^2	$=\text{C}_c\text{H}-$ -1.6 (A18)	1.92 (B18)
cyclic quaternary sp^2	$=\text{C}_c(\text{R})-$ -12.3 (A19)	
cyclic quaternary sp	$=\text{C}_c=$; $\text{R}-\text{C}_c\equiv$ -4.7 (A20)	

TABLE 2. (a) Contributions of the functional group portion of the molecule

Functional groups ^a	Group value (G_k) ^a J/(mol K)		Group coefficient (C_k) ^b				
			k				
			2	3	4	5	6
bromine	R-Br	17.5 (A21)					
chlorine	R-Cl	10.8 (A22)	1.5 (B22)	1.5 (C22)	1.5 (D22)	1.5 (E22)	1.5 (F22)
fluorine on an sp^2 carbon	=CRF	19.5 (A23)					
fluorine on an aromatic carbon	=CF-	16.6 (A24)					
3-fluorines on an sp^3 carbon	CF ₃ -R	13.3 (A25)					
2-fluorines on an sp^3 carbon	R-CF ₂ -R	16.4 (A26)					
1-fluorine on an sp^3 carbon	R-CF-(R) ₂	12.7 (A27)					
fluorine on a ring carbon	-CHF-	[17.5] (A28)					
	-CF ₂ -	[17.5] (A28)					
iodine	R-I	19.4 (A29)					
hydroxyl group	R-OH	1.7 (A30)	10.4 (B30)	9.7 (C30)	13.1 (D30)	12.1 (E30)	13.1 (F30)
phenol	=C-(OH)-	20.3 (A31)					
ether	R-O-R	4.71 (A32)					
peroxide, 1	R-O-O-R	[10.6] (A33)					
aldehyde	R-CH(=O)	21.5 (A34)					
ketone	R-C(=O)-(R)	4.6 (A35)					
carboxylic acid	R-C(=O)OH	13.4 (A36)	1.21 (B36)	2.25 (C36)	2.25 (D36)	2.25 (E36)	2.25 (F36)
formate ester	R-OCH(=O)	[4.2] (A37)					
ester	R-C(=O)O-R	7.7 (A38)					
anhydride	R-C(=O)OC(=O)-R	[10.0] (A39)					
acyl chloride	R-C(=O)Cl	[25.8] (A40)					
aromatic heterocyclic amine	=N-	[10.9] (A41)					
acyclic sp^2 nitrogen	=N-	[-1.8] (A42)					
tertiary amine	R-N(R) ₂	-22.2 (A43)					
secondary amine	R-NH-R	-5.3 (A44)					
primary amine	R-NH ₂	21.4 (A45)					
azide	R-N ₃	[-32.5] (A46)					
tertiary amine <i>N</i> -nitro	R ₂ -N-(NO ₂)	5.39 (A47)					
aliphatic secondary amine <i>N</i> -nitro	R-NH-(NO ₂)	[-4.59] (A48)					
aromatic tertiary amine- <i>N</i> -nitro	R-NH-(NO ₂)	[-41.7] (A49)					
nitro group	R-NO ₂	17.7 (A50)					
<i>N</i> -nitro	>N-(NO ₂)	39.8 (A51)					
<i>N</i> -nitroso	>N-N=O	[28.6] (A52)					
oxime	=N-OH	[13.6] (A53)					
azoxy nitrogen	N=N(→O)-	[6.8] (A54)					
nitrate ester	R-ONO ₂	[24.4] (A55)					
nitrile	R-C≡N	17.7 (A56)					
isocyanide	R-NC	[17.5] (A57)					
isocyanate	R-N=C=O	[23.1] (A58)					
tertiary amides	R-C(=O)NR ₂	-11.2 (A59)					
secondary amides	R-C(=O)NH-R	1.5 (A60)					
primary amide	R-CONH ₂	27.9 (A61)					
<i>N,N</i> -dialkylformamide, 1	HC(=O)NR ₂	[6.9] (A62)					
tetra substituted urea	R ₂ NC(=O)NR ₂	[-19.3] (A63)					
1,1,3-trisubst urea	R ₂ NC(=O)NH-R	[0.2] (A64)	-12.8 (B64)	-24 (C64)	6 (D64)		
1,1-disubstituted urea	R ₂ NC(=O)NH ₂	[19.5] (A65)					
1,3-disubstituted urea	RNHC(=O)NH-R	[1.5] (A66)					
mono substituted urea	R-NHC(=O)NH ₂	[22.5] (A67)					
<i>N,N</i> -disubstituted carbamate	R-OC(=O)NR ₂	-23.12 (A68)					
<i>N</i> -substituted carbamate	R-OC(=O)NH-R	10.6 (A69)					
carbamate	R-OC(=O)NH ₂	[27.9] (A70)					
imide	R-C(=O)NHC(=O)-R	[7.7] (A71)					
phosphine	R ₃ -P	[-20.7] (A72)					
phosphine oxide	R ₃ -P=O	[-32.7] (A73)					
phosphate ester	P(=O)(O-R) ₄	[-10.0] (A74)					
phosphonate ester	R-P(=O)(O-R) ₂	[-14.0] (A75)					
phosphonic acid	R-P=O(OH) ₂	[7.7] (A76)					
phosphonyl halide	R-P(=O)X ₂	[4.8] (A77)					

TABLE 2. (a) Contributions of the functional group portion of the molecule—Continued

Functional groups ^a	Group value (G_k) ^a J/(mol K)	Group coefficient (C_k) ^b				
		2	3	4	5	6
phosphoramidate ester	(R-O) ₂ P(=O)NH-R	[-0.7]				(A78)
phosphorothioate ester	(R-O) ₃ P(=S)	1.1				(A79)
phosphorodithioate ester	R-S-P(=S)(O-R) ₂	-9.6				(A80)
phosphonothioate ester	R-P(=S)(O-R) ₂	[5.2]				(A81)
phosphoroamidothioate ester	R-NHP(=S)(O-R) ₂	[16.0]				(A82)
phosphoroamidodithioate ester	NH ₂ P(=S)(S-R)(O-R)	[6.9]				(A83)
sulfides	R-S-R	2.1				(A84)
disulfides	R-SS-R	9.6				(A85)
thiols	R-SH	23.0				(A86)
sulfoxide	R-S(→O)-R	[14.1]				(A87)
sulfones	R-S(→O) ₂ -R	0.3				(A88)
sulfonate ester	R-S(→O) ₂ O-R	[7.9]				(A89)
1,2-disubstituted thiourea	R-NHC(=S)NH-R	[14.4]				(A90)
monosubst thiourea	R-NHC(=S)+NH ₂	[23.1]				(A91)
thioamide	R-C(=S)NH ₂	[30.0]				(A92)
N,N disubstituted thiocarbamate	R-S(C=O)N-R ₂	[5.6]				(A93)
N,N-disubstituted sulfonamide	R-S(→O) ₂ N-R ₂	[-11.3]				(A94)
N-substituted sulfonamide	R-S(→O) ₂ NH-R	6.3				(A95)
sulfonic acid	R-S(→O) ₂ OH	[1.8]				(A145)
sulfonamide	R-S(→O) ₂ NH ₂	[28.4]				(A96)
trisubstituted aluminum	R ₃ -Al	[-24.7]				(A97)
trisubstituted arsenic	R ₃ -As	[-6.5]				(A98)
trisubstituted boron	R ₃ -B	[-17.2]				(A99)
trisubstituted bismuth	R ₃ -Bi	[-14.5]				(A100)
trisubstituted gallium	R ₃ -Ga	[-11.9]				(A101)
tetrasubstituted germanium	R ₄ -Ge	[-35.2]				(A102)
disubstituted germanium	R ₂ GeH ₂	[-14.7]				(A103)
disubstituted mercury	R ₂ -Hg	[8.4]				(A104)
trisubstituted indium	R ₃ -In	[-19.3]				(A105)
tetrasubstituted lead	R ₄ -Pb	[-30.2]				(A106)
trisubstituted antimony	R ₃ -Sb	[-12.7]				(A107)
disubstituted selenium	R ₂ -Se	[6.0]				(A108)
quaternary silicon	R ₄ -Si	-27.1				(A109)
quaternary tin	R ₄ -Sn	-24.2				(A110)
disubstituted zinc	R ₂ -Zn	[11.1]				(A111)
disubstituted telluride	R ₂ -Te	[-2.2]				(A140)
trisubstituted germanium	R ₃ -GeH	[-27.8]				(A141)
disubstituted arsenic acid	R ₂ -AsO ₂ H	[-24]				(A142)
trisubstituted thallium	R ₃ -Th	[1]				(A143)
disubstituted cadmium	R ₂ -Cd	[-2]				(A144)

^aR: any alkyl or aryl group unless specified otherwise; X: any halogen; units: J mol⁻¹ K⁻¹.

^bUnassigned values beneath each of the group coefficients; C_k can be assumed to be 1.



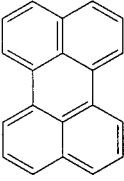

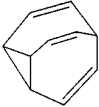

TABLE 2. (b) Contributions of functional groups as part of a ring

Heteroatoms and functional groups comprising a portion of a ring ^b		Group value (G_k) ^a	
cyclic ether	$R-O-R$	1.2	(A112)
cyclic peroxide	$R-OO-R$	[27.7]	(A113)
cyclic ketone	$R-C(=O)-R$	-1.4	(A114)
cyclic ester	$R-C(=O)O-R$	3.1	(A115)
cyclic carbonate	$R-OC(=O)O-R$	[1.3]	(A116)
cyclic anhydride	$R-C(=O)-O-C(=O)-R$	2.3	(A117)
cyclic sp^2 nitrogen	$R=N-R$	0.5	(A118)
cyclic tertiary amine	$R_2>N-R$	-19.3	(A119)
cyclic tertiary amine-N-nitro,	$R_2>N-(NO_2)-R$	-27.1	(A120)
cyclic tertiary amine-N-nitroso	$R_2>N-(N=O)-R$	-27.1	(A120)
cyclic secondary amine	$R_2>NH$	2.2	(A121)
cyclic tertiary amine N-oxide	$R_2>N(-O)-R$	[-22.2]	(A122)
cyclic azoxy group	$R=N(-O)-R$	[2.9]	(A123)
cyclic sec amide	$R-C(=O)NH-R$	2.7	(A124)
cyclic tertiary amide	$R-C(=O)N<RR$	-21.7	(A125)
cyclic tertiary amide	$R-C(=O)N<R_2$	[-9]	(A146)
cyclic carbamate	$R-OC(=O)N-RR$	[-5.2]	(A126)
cyclic carbamate	$R-OC(=O)N-HR$	[19.7]	(A125)
cyclic urea	$R-NC(=O)N<RR$	[-40.6]	(A127)
N-substituted cyclic imide	$R-C(=O)N(R)C(=O)-R$	[1.1]	(A128)
cyclic imide	$R-C(=O)N(H)C(=O)-R$	[1.4]	(A129)
cyclic phosphorothioate	$R-O-P(=S)<(OR)(OR)$	[-15.6]	(A130)
cyclic sulfide	$R-S-R$	2.9	(A131)
cyclic disulfide	$R-SS-R$	[-6.4]	(A132)
cyclic disulfide S-oxide	$R-SS(-O)-R$	[1.9]	(A133)
cyclic sulphone	$R-S(-O)_2-R$	[-10.4]	(A134)
cyclic thiocarbonate	$R-OC(=O)S-R$	[14.2]	(A135)
cyclic sulfate	$R-OS(-O)_2O-R$	0.9	(A136)
cyclic N-substituted sulphonamide	$R-S(-O)_2NH-R$	[-0.4]	(A137)
cyclic thiocarbamate	$R-S-(C=O)NHR$	[13.9]	(A138)
cyclic quaternary silicon	$R_2>Si<R_2$	-34.7	(A139)

^aR: any alkyl or aryl group unless specified otherwise; values in brackets are tentative assignments; units: $J mol^{-1} K^{-1}$.

^bThe R groups that are a part of the ring structure are designated by italics.

TABLE 3. Estimations of total phase change entropies and enthalpies of hydrocarbons^a

C_8H_8 styrene ^b 		C_7H_{14} 1-heptene ^b 	
$T_{fus}:$ 242.3 K $\Delta_0^{fus} S_{tpce}:$ 52.2 (45.2) $\Delta_0^{fus} H_{tpce}:$ 12.6 (11.0) $\Delta_0^{fus} S_{tpce}:$ {5[7.4]+[-7.5]+[5.3]+[17.3]}		$T_{fus}:$ 154.3 K $\Delta_0^{fus} S_{tpce}:$ 77.5 (81.) $\Delta_0^{fus} H_{tpce}:$ 12.0 (12.6) $\Delta_0^{fus} S_{tpce}:$ {[17.3]+[5.3]+4[1.31][7.1]+17.6]}	
$C_{20}H_{12}$ perylene ^b 		$C_{20}H_{32}$ 10,10,13,13-tetramethyl-1,5-cyclohexadecadiene ^c 	
$T_{fus}:$ 551 K $\Delta_0^{fus} S_{tpce}:$ 42.4 (57.9) $\Delta_0^{fus} H_{tpce}:$ 23.4 (31.9) $\Delta_0^{fus} S_{tpce}:$ {12[7.4]+6[-7.5]+2[-0.7]}		$T_{fus}:$ 323 K $\Delta_0^{fus} S_{tpce}:$ 63.8 (58.3) $\Delta_0^{fus} H_{tpce}:$ 20.6 (18.8) $\Delta_0^{fus} S_{tpce}:$ {[33.4]+13[3.7]+4[17.6]+2[-34.6]4[-4.7]}	
$C_{10}H_{10}$ bullvalene ^b 		$C_{12}H_8$ acenaphthylene ^{b,d} 	
$T_{fus}:$ 366.5 K $\Delta_0^{fus} S_{tpce}:$ 35.3 (41.6) $\Delta_0^{fus} H_{tpce}:$ 12.9 (15.3) $\Delta_0^{fus} S_{tpce}:$ {3[33.4]+[3.7]6[-1.6]+4[-14.7]}		$T_1:$ 116.6; 127.1 K $T_{fus}:$ 362.6 K $\Delta_0^{fus} S_{tpce}:$ 37.6 (12.1+19.1) $\Delta_0^{fus} H_{tpce}:$ 13.6 (1.5+6.9) $\Delta_0^{fus} S_{tpce}:$ {[33.4]+2[3.7]+[-7.5]+6[7.4]+3[-12.3]+2[-1.6]}	

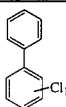
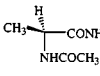

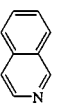
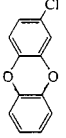
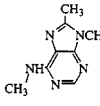
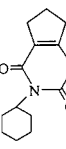
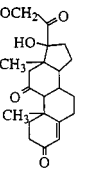
^aUnits for $\Delta_0^{fus} S_{tpce}$ and $\Delta_0^{fus} H_{tpce}$ are $J \cdot mol^{-1} \cdot K^{-1}$ and $kJ \cdot mol^{-1}$, respectively; experimental values are included in parentheses following the calculated value (in cases where additional solid–solid transitions are involved, the first term given is the total property associated with the transition(s) and the second term represents the fusion property).

^bReference 11.

^cReference 12.

^dReference 13.

TABLE 4. Estimations of total phase change entropies and enthalpies

A. Substituted Aromatic and Aliphatic Molecules ^a			
$C_{17}Cl_{10}$ decachlorobiphenyl ^c 		$C_5H_{10}N_2O_2$ N-acetyl-L-alanine amide ^c 	
$T_{fus}:$ 577.7 K $\Delta_0^{fus} S_{tpce}:$ 72.1 (68.1) $\Delta_0^{fus} H_{tpce}:$ 41.6 (39.3) $\Delta_0^{fus} S_{tpce}:$ {12[-7.5]+10[1.5][10.8]}		$T_{fus}:$ 431 K $\Delta_0^{fus} S_{tpce}:$ 54.9 (50.4) $\Delta_0^{fus} H_{tpce}:$ 23.7 (21.7) $\Delta_0^{fus} S_{tpce}:$ {2[17.6]+[27.9]+0.6[-16.4]+[1.5]}	
C_2F_3N 2,2,2-trifluoroacetone nitrile ^c 		C_9H_7N isoquinoline ^c 	
$T_{fus}:$ 128.7 K $\Delta_0^{fus} S_{tpce}:$ 34.6 (38.6) $\Delta_0^{fus} H_{tpce}:$ 4.5 (5.0) $\Delta_0^{fus} S_{tpce}:$ {[[-34.8][0.66]3[13.3]+[17.7]}		$T_{fus}:$ 299.6 K $\Delta_0^{fus} S_{tpce}:$ 47.9 (52.1) $\Delta_0^{fus} H_{tpce}:$ 14.3 (13.5) $\Delta_0^{fus} S_{tpce}:$ {[110.9]+7[7.4]+2[-7.5]}	
B. Substituted Cyclic Molecules ^a			
$C_{17}H_7ClO_2$ 2-chlorodibenzodioxin ^d 		$C_8H_{11}N_5$ 6,8,9-trimethyladenine ^e 	
$T_{fus}:$ 362.2 K $\Delta_0^{fus} S_{tpce}:$ 58.5 (63.8) $\Delta_0^{fus} H_{tpce}:$ 21.2 (23.1) $\Delta_0^{fus} S_{tpce}:$ {[33.4]+3[3.7]+2[1.2]+4[-12.3]+7[7.4]+[-7.5]+[1.5][10.8]}		$T_{fus}:$ 438 K $\Delta_0^{fus} S_{tpce}:$ 54.3 (52.7) $\Delta_0^{fus} H_{tpce}:$ 23.8 (23.1) $\Delta_0^{fus} S_{tpce}:$ {[33.4]+2[3.7]3[17.6]+2[10.9]+[0.5]+[-19.3]+[-5.3]+[-7.5]+[7.4]+3[-12.3]}	
$C_{17}H_{18}N_2O_2$ Lenacil ^g 		$C_{21}H_{28}O_5$ cortisone ^f 	
$T_{fus}:$ 584.3 K $\Delta_0^{fus} S_{tpce}:$ 64.0(72.4) $\Delta_0^{fus} H_{tpce}:$ 37.4 (42.3) $\Delta_0^{fus} S_{tpce}:$ {3[33.4]+6[3.7]+2[-12.3]+[-14.7]+[-21.7][2.7]}		$T_{fus}:$ 495 K $\Delta_0^{fus} S_{tpce}:$ 75.2 (74.5) $\Delta_0^{fus} H_{tpce}:$ 37.2 (36.9) $\Delta_0^{fus} S_{tpce}:$ {[4[33.4]+5[3.7]+[4.6]+2[17.6]+[7.1]+[-12.3]+[-1.6][1.92]+2[-1.4]+3[-14.7]+3[-14.7]+3[-34.6]+2[1.7][12.1]}	

^aUnits for $\Delta_0^{fus} S_{tpce}$ and $\Delta_0^{fus} H_{tpce}$ are $J \cdot mol^{-1} \cdot K^{-1}$ and $kJ \cdot mol^{-1}$, respectively; experimental values are given in parentheses.

^bReference 14.

^cReference 11.

^dReference 15.

^eReference 16.

^fReference 17.

^gReference 18.

TABLE 5. Experimental and calculated total phase change enthalpy and entropy of database^a

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
CBrCl ₃		bromotrichloromethane				
	238.2	4.62	19.4			
	259.3	0.53	2.03			
	267.9	2.03	7.58	29.0	43.2	7.2
	A4*B4+A21+3*A22*D22					
CBr ₄		carbon tetrabromide				
	320	5.94	18.58			
	363.2	3.95	10.88	29.46	47.3	9.9
	A4*B4+4*A21					
CCl ₃ F		fluorotrichloromethane				
	162.7	6.9	0	42.38	38.4	6.9
	A4*B4+3*A22*D22+A27					
CCl ₄		carbon tetrachloride				
	224.6	4.6	20.49			
	249	2.69	10.82	31.31	41.9	7.3
	225.4	4.58	20.3			
	250.3	2.52	10.1	30.4		7.1
	225.7	4.63	20.5			
	250.5	2.56	10.2	30.7		7.2
	4*A22*D22+A4*B4					
CF ₄		carbon tetrafluoride				
	76.27	1.71	22.43			
	89.56	0.71	7.95	30.38	30.1	2.42
	76.1	1.73	21.4			
	88.4	0.69	7.7	29.1		2.4
	76.1	1.46	19.2			
89.5	0.71	7.9	27.1		2.2	
	4*A25+A4*B4					
CHClF ₂		chlorodifluoromethane				
	59	0.07	1.13			
	115.7	4.12	35.65	36.78	39.3	4.19
	2*A26+A3*B3+A22*B22					
CHCl ₃		trichloromethane				
	209.6	8.8	0	41.98	38.9	8.8
	A3*B3+3*A22*C22					
CHF ₃		trifluoromethane				
	118.0	4.06	0	34.85	30.5	4.06
	3*A25+A3*B3					
CHF ₃ S		trifluoromethanethiol				
	116.0	4.93	0	42.44	39.9	4.93
	3*A25+A4*B4+A86					
CH ₂ Cl ₂		dichloromethane				
	178.2	6.16	0	34.56	39.5	6.16
	A2+2*A22*B22					
CH ₂ N ₂		cyanamide				
	317.2	8.76	0	27.62	39.1	8.76
	318.7	7.27	0	22.8		7.27
	A56+A45					
CH ₂ N ₄		tetrazole				
	432.1	17.7	0	40.96	41.5	17.7
	430.7	18.4	0	42.7		18.4
	242.5	0.014	0.06			
	430	18.0	41.9	42.0		18.14
	A14+2*A15+A121+3*A118+A18*B18					
CH ₃ Br		bromomethane				
	173.8	0.47	2.72			
	179.5	5.98	3.33	36.02	35.1	6.45
	A21+A1					
CH ₃ Cl		methyl chloride				
	174.5	6.43	0	36.82	28.4	6.42
	A1+A22					
CH ₃ CIFOP		methylphosphonyl chlorofluoride				
	250.7	11.85	0	47.28	51.2	11.85
		A1+A22*C22+A27+A77				

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)	
CH ₃ Cl ₂ OP	306.1	methylphosphonyl dichloride 18.08	0	59.05	54.8	18.08	16.8
		A1 + 2*A22*C22 + A77					[94]
CH ₃ Cl ₃ Si	197.4	trichloromethylsilane 8.95	0	45.32	39.1	8.95	7.7
		3*A22*D22 + A1 + A109					[216]
CH ₃ F ₂ OP	236.3	methylphosphonyl difluoride 11.88	0	50.27	55.1	11.8	13.0
		A1 + 2*A26 + A77					[94]
CH ₃ NO	275.7	formamide 7.98	0	28.94	27.9	7.98	7.7
	275.6	8.67	0	31.5		8.67	
		A61					[216]
CH ₃ NO ₂	244.8	nitromethane 9.7	0	39.62	35.3	9.7	8.64
		A1 + A50					[216]
CH ₃ NO ₃	190.2	methyl nitrate 8.24	0	43.33	42.0	8.24	8.0
		A1 + A55					[216]
CH ₄ O	161.1	methanol 0.59	3.7				
	175.3	3.18	18.1	21.8	19.3	3.77	3.4
	157.3	0.64	4.0				
	175.6	3.22	18.3	22.3		3.86	
		A1 + A30					[216]
CH ₄ N ₄ O ₄	371	N,N'-dinitro-diaminomethane 35.85	0	96.63	77.5	35.85	28.7
		A2 + 2*A51 + 2*A48					[225]
CH ₄ S	137.6	methanethiol 2.2	1.59				
	150.2	5.9	39.33	40.92	40.6	8.1	6.1
		A1 + A86					[216]
CH ₅ N	179.7	methylamine 6.13	0	34.14	38.9	6.13	7.0
		A1 + A45					[216]
CH ₆ N ₂	220.8	methylhydrazine 10.42	0	47.19	33.7	10.42	7.4
		A1 + A44 + A45					[216]
C ₂ Br ₂ F ₂	162.8	dibromodifluoroethylene 7.04	0	43.22	52.6	7.04	8.6
		2*A21 + 2*A23 + 2*A7					[216]
C ₂ Br ₂ F ₄	162.8	1,2-dibromotetrafluoroethane 7.04	0	43.24	54.9	7.04	8.9
		2*A4*B4 + 2*A21 + 4*A26					[215]
C ₂ ClF ₃	115	chlorotrifluoroethylene 5.55	0	48.28	53.2	5.55	6.1
		2*A7 + 3*A23 + A22*B22					[216]
C ₂ ClF ₅	80.24	perfluorochloroethane 2.63	32.76				
	173.7	1.88	10.79	43.56	42.9	4.51	7.5
		2*A26 + 2*A4*B4 + A22*B22 + 3*A25					[216]
C ₂ Cl ₂ F ₄	109.3	1,2-dichloro-tetrafluoroethane 1.21	11.1				
	134.6	2.63	19.52				
	180.6	1.51	8.36	39.0	52.1	5.35	9.4
		2*A22*C22 + 4*A26 + 2*A4*B4					[216]
C ₂ Cl ₃ F ₃	82.5	1,1,2-trifluoro-1,2,2-trichloroethane 0.83	10.08				
	236.9	2.47	10.42	20.5	48.2	3.3	11.4
		3*A22*D22 + 2*A26 + 2*A4*B4 + A27					[215]
C ₂ Cl ₄	210	tetrachloroethene 0.82	3.9				
	250.8	10.88	43.38	47.28	43.3	11.7	10.9
		4*A22*D22 + 2*A7					[216]
C ₂ Cl ₄ F ₂	130	1,1,2,2-tetrachlorodifluoroethane 0.79	6.08				
	299.7	3.7	12.35	18.42	44.3	4.49	13.3

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C_2N_2	245.3	4*A22*E22+2*A27+2*A4*B4 cyanogen 8.11	0	33.05	8.11	[215,158] 8.7
C_2Cl_6	318	2*A56 hexachloroethane 2.57	8.07			[216]
	345	8.22	23.83			
	458	9.75	21.29	53.18	20.54	23.5
C_2F_3N	128.7	6*A22*F22+2*A4*B4 trifluoroacetone 4.97	0	38.62	4.97	[216] 4.5
C_2F_4	142	3*A25+A4*B4+A56 tetrafluoroethylene 7.71	0	54.31	7.71	[216] 8.0
C_2F_6	104.0	4*A23+2*A7 hexafluoroethane 3.74	35.9			[216]
	173.1	2.69	15.5	51.4	6.0	6.0
$C_2HBrClF_3$	154.7	6*A25+2*A4*B4 2-bromo-2-chloro-1,1,1-trifluoroethane 4.84	0	31.29	4.84	[216] 6.3
$C_2HBrClF_3$	146.2	A22*C22+A21+3*A25+A4*B4+A3*B3 1-bromo-2-chloro-1,1,2-trifluoroethane 4.38	0	29.96	4.38	[216] 6.8
C_2HCl_3	188.5	A22*C22+A21+2*A26+A4*B4+A3*B3+A27 trichloroethylene 8.45	0	44.83	8.45	[216] 7.9
$C_2HCl_3O_2$	330.7	3*A22*C22+A6*B6+A7 trichloroacetic acid 5.88	0	17.78	5.88	[215] 18.4
$C_2H_2Br_2F_2$	206.3	3*A22*D22+A36*D36+A4*B4 1,2-dibromo-1,1-difluoroethane 8.3	0	40.23	8.3	[215] 10.8
$C_2H_2Cl_2$	150.9	2*A21+2*A26+A2+A4*B4 1,1-dichloroethene 6.51	0	43.26	6.51	[216] 5.9
$C_2H_2Cl_2F_2$	163.0	2*B22*A22+A7+A5 1,2-difluoro-2,2-dichloroethane 8.19	0	50.26	8.19	[216] 6.8
$C_2H_2Cl_2O_2$	286.5	2*A22*C22+A4*B4+2*A27+A2 dichloroacetic acid 12.34	0	43.08	12.34	[216] 15.1
$C_2H_2Cl_4$	207.3	2*A22*C22+A3*B3+A36*C36 1,1,2,2-tetrachloroethane 0.54	2.62			[216]
	230.8	9.17	39.74	42.38	9.72	10.5
	204.8	0.36	1.74			
	230.3	9.52	41.5	43.2	9.88	
$C_2H_3Br_3$	244	2*A3*B3+4*A22*D22 1,1,2-tribromoethane 9.11	0	37.34	9.11	[215] 12.2
C_2H_3Cl	119.3	A2+A3*B3+3*A21 vinyl chloride 4.92	0	41.21	4.92	[216] 3.8
$C_2H_3ClF_2$	142.4	A5+A6*B6+A22 1,1-difluoro-1-chloroethane 2.69	0	18.86	2.69	[216] 6.2
$C_2H_3ClO_2$	334.3	2*A26+A22*B22+A1+A4*B4 (α form) chloroacetic acid 16.3	0	48.74	16.3	[216] 13.2
$C_2H_3ClO_2$	329.2	A22*B22+A2+A36*B36 (β form) chloroacetic acid 13.93	0	42.33	13.93	[216] 13.0
$C_2H_3Cl_3$	237.1	A22*B22+A2+A36*B36 1,1,2-trichloroethane 11.38	0	48	11.38	[216] 10.9
	237.9	10.9	0	45.7	10.9	
$C_2H_3Cl_3$		3*A22*C22+A2+A3*B3 1,1,1-trichloroethane				[74]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
205	0.21	1.02				
223.6	7.45	33.31				
240.1	1.88	7.84	42.17	43.3	9.54	10.4
224.2	7.47	33.3				
240.2	1.88	7.8	41.1		9.4	
224.8	7.49	33.3				
243.1	2.35	9.67	43.0		9.8	
$\text{C}_2\text{H}_3\text{F}_3$	3*A22*C22+A4*B4+A1					[216]
	1,1,1-trifluoroethane					
161.9	6.19	0	38.23	34.5	6.19	5.6
156.4	0.3	1.9				
161.8	6.19	38.3	40.2		6.39	
$\text{C}_2\text{H}_3\text{N}$	3*A25+A4*B4+A1					[215]
	acetonitrile					
216.9	0.9	4.14				
229.3	8.17	35.61	39.75	35.3	9.06	8.1
$\text{C}_2\text{H}_3\text{N}_3$	A1+A56					[216]
	1,2,4-triazole					
393.5	16.1	0	40.91	37.8	16.1	14.9
C_4H_4	A14+2*A15+2*A118+A121+2*A18*B18					[216]
	ethylene					
104.0	3.35	0	32.24	34.7	3.35	3.6
$\text{C}_2\text{H}_4\text{BrCl}$	2*A5					[216]
	1-bromo-2-chloroethane					
182	3.1	17.15				
256.4	9.62	37.53	54.69	48.0	12.72	12.3
$\text{C}_2\text{H}_4\text{Br}_2$	2*A2+A21+A22*B22					[216]
	1,2-dibromoethane					
249.5	1.94	7.78				
283	10.94	38.66	46.44	49.4	12.88	14.0
$\text{C}_2\text{H}_4\text{Cl}_2$	2*A21+2*A2					[216]
	1,1-dichloroethane					
176.2	7.87	0	44.77	40.3	7.87	7.1
$\text{C}_2\text{H}_4\text{Cl}_2$	2*B22*A22+A1+A3*B3					[215]
	1,2-dichloroethane					
237.2	8.83	0	37.24	46.6	8.83	11.1
175	2.85	16.2				
237.6	8.75	36.8	53.0		11.6	
$\text{C}_2\text{H}_4\text{D}_2\text{O}_2$	2*A22*B22+2*A2					[216]
	dihydroxyethane- d_2					
258.8	9.75	0	37.67	50.5	9.75	13.1
$\text{C}_2\text{H}_4\text{N}_4$	2*A2+2*A30*B30					[55]
	1H-1,2,4-triazol-3-amine					
428.3	21.93	0	51.2	52.2	21.93	22.4
$\text{C}_2\text{H}_4\text{N}_4$	A14+2*A15+2*A121+2*A118+A18*B18+A19+A45					[221]
	1-methyltetrazole					
315	15.7	0	49.85	37.5	15.7	11.8
$\text{C}_2\text{H}_4\text{N}_4$	A14+2*A15+A119+3*A118+A1+A18*B18					[174]
	2-methyltetrazole					
286	12.37	0	43.25	37.5	12.37	10.7
$\text{C}_2\text{H}_4\text{N}_4$	A14+2*A15+A119+3*A118+A1+A18*B18					[174]
	5-methyltetrazole					
418	16	0	38.28	49.9	16	20.8
$\text{C}_2\text{H}_4\text{O}$	A14+2*A15+3*A118+A121+A1+A19					[174]
	ethylene oxide					
160.7	5.17	0	32.22	34.6	5.17	5.6
$\text{C}_2\text{H}_4\text{O}$	A14+A112					[216]
	acetaldehyde					
149.8	2.31	15.42				
242.9	1.72	7.06	22.49	39.1	4.03	9.5
$\text{C}_2\text{H}_4\text{O}_2$	A1+A34					[216]
	ethanoic acid					
298.7	11.72	0	39.24	31.0	11.72	9.2
$\text{C}_2\text{H}_5\text{Cl}$	A36+A1					[216]
	chloroethane					
134.8	4.45	0	33.01	35.5	4.45	4.8
$\text{C}_2\text{H}_5\text{Cl}_3\text{Si}$	A22+A2+A1					[215]
	ethyltrichlorosilane					
165.3	6.96	0	42.1	46.2	6.96	7.6
$\text{C}_2\text{H}_5\text{NO}$	A1+A2+3*A22*C22+A109					[216]
	acetamide					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
353	15.6	0	44.19	45.5	15.6	16.1
354	15.5	0	43.8		15.5	
$\text{C}_2\text{H}_5\text{NO}_2$	A1 + A61					[271,216]
	nitroethane					
183.7	9.85	0	53.64	42.4	9.85	7.8
$\text{C}_2\text{H}_5\text{NO}_2$	A1 + A2 + A50					[216]
	methyl carbamate					
328.6	16.7	0	50.82	45.5	16.7	14.9
$\text{C}_2\text{H}_5\text{NO}_3$	A1 + A70					[216]
	ethyl nitrate					
178.6	8.53	0	47.74	49.1	8.53	8.8
$\text{C}_2\text{H}_5\text{NS}$	A1 + A2 + A55					[126]
	ethanethioamide					
385.7	18.36	0	47.59	47.6	18.36	18.4
C_2H_6	A1 + A92					[221]
	ethane					
89.5	2.79	0	31.21	35.2	2.79	3.2
89.9	2.86	0	31.8		2.86	
$\text{C}_2\text{H}_6\text{ClO}_3\text{P}$	2*A1					[216]
	2-chloroethylphosphonic acid					
347.9	14.79	0	42.51	42.6	14.79	14.8
$\text{C}_2\text{H}_6\text{Cl}_2\text{Si}$	2*A2 + A22*B22 + A76					[221]
	dimethyldichlorosilane					
199.0	8.83	0	44.36	40.5	8.83	8.1
$\text{C}_2\text{H}_6\text{N}_2\text{O}$	2*A1 + 2*A22*C22 + A109					[216]
	N-methylurea					
378.1	14.06	0	37.19	40.09	14.06	15.16
373.8	15.75		42.1		15.75	
$\text{C}_2\text{H}_6\text{N}_2\text{O}_2$	A1 + A67					[138,216]
	N-nitro-N-methylaminomethane					
327	37.66	0	115.16	80.3	37.66	26.3
$\text{C}_2\text{H}_6\text{N}_4\text{O}_4$	2*A1 + A51 + A47					[225]
	N,N'-dinitroethanediamine					
450	29.5	0	65.55	84.6	29.5	38.07
$\text{C}_2\text{H}_6\text{O}$	2*A2 + 2*A48 + 2*A51					[225]
	ethanol					
111.4	3.14	28.16				
158.8	4.64	29.25	57.4	26.46	7.78	4.2
127.5	0.66	5.2				
159	4.93	31.0	36.2		5.6	
$\text{C}_2\text{H}_6\text{O}$	A1 + A2 + A30					[216]
	dimethyl ether					
131.7	4.94	0	37.5	39.9	4.94	5.3
$\text{C}_2\text{H}_6\text{OS}$	2*A1 + A32					[216]
	dimethyl sulfoxide					
291.7	14.37	0	49.26	49.3	14.37	14.4
$\text{C}_2\text{H}_6\text{O}_2$	2*A1 + A87					[216]
	dihydroxyethane					
260.6	9.96	0	38.21	50.5	9.96	13.2
260.8	11.6	0	44.6		11.6	
$\text{C}_2\text{H}_6\text{O}_2\text{S}$	2*A2 + 2*A30*B30					[216]
	dimethylsulfone					
382	18.28	0	47.91	35.4	18.30	13.5
$\text{C}_2\text{H}_6\text{S}$	2*A1 + A88					[216]
	ethyl mercaptan					
195.3	4.97	0	25.48	47.7	4.97	9.3
$\text{C}_2\text{H}_6\text{S}$	A1 + A2 + A86					[216]
	dimethyl sulfide					
174.9	7.98	0	45.66	37.3	7.98	6.5
$\text{C}_2\text{H}_6\text{S}_2$	2*A1 + A84					[216]
	dimethyldisulfide					
188.4	9.19	0	48.78	44.7	9.19	8.4
$\text{C}_2\text{H}_6\text{Se}$	2*A1 + A85					[216]
	dimethylselenium					
185.1	8.5	0	45.91	41.1	8.5	7.6
$\text{C}_2\text{H}_6\text{Se}_2$	2*A1 + A108					[170]
	dimethyldiselenium					
190.8	8.55	0	44.78	47.1	8.55	9.0
	2*A1 + 2*A108					[170]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
C ₂ H ₆ Zn	210.3	dimethyl zinc 1.06	5.05			
	230.1	6.83	29.68	34.73	46.2	7.89
C ₂ H ₇ AsO ₂	470.9	2*A1 + A111 hydroxydimethyl arsine 24.46	0	51.93	46.8	24.46
		2*A1 + A98 + A30*B30 dimethyl amine 5.94	0	29.68	29.9	5.94
C ₂ H ₈ NOPS ₂	316.8	2*A1 + A44 O,S-dimethyl phosphoroamidothioate 13.34	0	42.1	42.1	13.34
		2*A1 + A83 diaminoethane 0.49	2.57			
C ₂ H ₈ N ₂	189.0 284.2	22.58	79.43	82.05	57.0	23.07
		2*A45 + 2*A2 N,N-dimethylhydrazine 10.07	0	46.64	34.3	10.07
C ₂ H ₈ N ₂	264.3	2*A1 + A45 + A43 N,N'-dimethylhydrazine 13.64	0	51.6	24.6	13.64
		2*A1 + 2*A44 hexachlorocyclopropane 18.6	49.47	49.47	26.8	18.6
C ₃ Cl ₆	376	6*A22*F22 + 3*A17 + A14 hexafluoroacetone 8.38	0	56.74	38.3	8.38
		6*A25 + 2*A4*B4 + A35 octafluoropropane 3.56	35.77			
C ₃ F ₆ O	147.7	0.48	3.81	39.58	43.6	4.03
		2*A26 + 3*A4*B4 + 6*A25 3-chloro-1,1,1,3,3-pentafluoropropane 10.47	0	63.3	50.07	10.47
C ₃ F ₈	99.4 125.5	2*A26 + A22*B22 + 2*A4*B4 + A2 + 3*A25 1,1,1-trichloro-3,3,3-trifluoropropane 14.07	0	60.46	49.71	14.07
		3*A22*D22 + 3*A25 + A2 + 2*A4*B4 dicyanomethane 10.8	0	35.4	42.59	10.8
C ₃ H ₂ ClF ₅	165.4	2*A56 + A2 1,1,1-trifluoro-3,3-dichloropropane 0.2	1.21			
		3*A25 + A4*B4 + A3*B3 + A2 + 2*A22C22 acrylonitrile 1.19	7.32			
C ₃ H ₂ Cl ₃ F ₃	232.7	6.23	32.84	40.17	39.0	7.42
		A5 + B6*A6 + A56 thiazole 9.58	40.08	40.04	35.0	9.58
C ₃ H ₃ N	162.5 189.6	A14 + 2*A15 + A131 + A118 + 3*A18*B18 s-triazine 0.07	0.37			
		3*A10 + 3*A41 1,1,1-trifluoro-3-chloropropane 4.49	26.44			
C ₃ H ₃ NS	239.4	5.05	28.2	54.6	47.3	9.54
		3*A25 + A4*B4 + 2*A2 + A22*B22 β -trichlorosilylpropionitrile 21.24	0	68.99	53.5	21.24
C ₃ H ₃ N ₃	197.7 353.4	2*A2 + A56 + 3*A22*E22 + A109 1,1,1,3-tetrachloropropane 2.2	10.03			
		4*A22*D22 + A4*B4 + 2*A2 imidazole 12.8	0	35.37	37.3	12.8
C ₃ H ₄ ClF ₃	169.8 179.3	10.49	44.13	54.16	56.2	12.69
		3*A25 + A4*B4 + 2*A2 + A22*B22 β -trichlorosilylpropionitrile 21.24	0	68.99	53.5	21.24
C ₃ H ₄ Cl ₃ NSi	307.9	2*A2 + A56 + 3*A22*E22 + A109 1,1,1,3-tetrachloropropane 2.2	10.03			
		4*A22*D22 + A4*B4 + 2*A2 imidazole 12.8	0	35.37	37.3	12.8
C ₃ H ₄ Cl ₄	219.9 237.7	10.49	44.13	54.16	56.2	12.69
		4*A22*D22 + A4*B4 + 2*A2 imidazole 12.8	0	35.37	37.3	12.8
C ₃ H ₄ N ₂	361.9	12.8	0	35.37	37.3	12.8
		12.8	0	35.37	37.3	12.8

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
$\text{C}_3\text{H}_4\text{N}_2$	343.2	$A14 + 2*A15 + 2*A18*B18 + A118 + A121$ pyrazole 14.2	0	41.38	14.2	[216] 12.8
$\text{C}_3\text{H}_4\text{N}_2\text{O}$	346.5 387.3	$A14 + 2*A15 + 2*A18*B18 + A118 + A121$ cyanoacetamide 1.2	3.46	59.49	22.9	[216] 20.4
$\text{C}_3\text{H}_4\text{O}_2$	285.5	$A2 + A56 + A61*B61$ acrylic acid 11.16	0	39.09	11.16	[216] 9.9
$\text{C}_3\text{H}_4\text{O}_2$	239.9	$A5 + A6*B6 + A36$ β -propiolactone 9.41	0	39.22	9.41	[215] 9.7
$\text{C}_3\text{H}_4\text{O}_3$	309.5	$A14 + A15 + A115$ ethylene carbonate 13.3	0	42.96	13.3	[32] 13.0
$\text{C}_3\text{H}_5\text{Br}_3$	289.4	$A14 + 2*A15 + A116$ 1,2,3-tribromopropane 23.78	0	82.17	23.78	[52] 16.6
$\text{C}_3\text{H}_5\text{N}$	177.0 180.4	$2*A2 + A3*B3 + 3*A21$ propionitrile 17.07	9.67	37.57	22.1	[215] 7.7
$\text{C}_3\text{H}_5\text{NO}$	358	$A1 + A2 + A56$ acrylamide 15.33	0	42.82	15.33	[216] 17.6
$\text{C}_3\text{H}_5\text{N}_3\text{O}_9$	285.5	$A5 + A6*B6 + A61$ trinitroglycerine 21.87	0	76.6	21.87	[216] 22.2
C_3H_6	88.2 87.85	$2*A2 + A3*B3 + 3*A55$ propene 2.93	0	33.3 34.18	2.93 3.0	[215] 3.5
C_3H_6	145.6	$A1 + A5 + A6$ cyclopropane 5.44	0	37.4	5.44	[216] 4.9
$\text{C}_3\text{H}_6\text{Br}_2$	238.6	$A14$ 1,3-dibromopropane 14.64	0	61.5	14.64	[216] 15.1
$\text{C}_3\text{H}_6\text{ClNO}_2$	213.8 261.6	$2*A21 + 3*A2*B2$ 2-chloro-2-nitropropane 9.54	44.62	49.72	10.88	[216] 12.1
$\text{C}_3\text{H}_6\text{Cl}_2$	172.7	$2*A1 + A4*B4 + A50 + A22*B22$ 1,2-dichloropropane 6.4	0	37.06	6.4	[216] 8.2
$\text{C}_3\text{H}_6\text{Cl}_2$	188 239.3	$A1 + A2 + A3*B3 + 2*A22*B22$ 2,2-dichloropropane 5.98	31.8	41.42	8.32	[215] 10.8
$\text{C}_3\text{H}_6\text{N}_2\text{O}_2$	393 443	$2*B22*A22 + 2*A1 + A4*B4$ malonamide 1.9	4.83	85.65	37.7	[216] 27.9
$\text{C}_3\text{H}_6\text{N}_2\text{O}_4$	267.7 259.7 324.5	$2*A61 + A2$ 2,2-dinitropropane 11.28	42.13	57.15	15.78	[292] 15.5
$\text{C}_3\text{H}_6\text{N}_4$	349	$2*A1 + A4*B4 + 2*A50$ 1,5-dimethyltetrazole 14.7	0	42.12	14.7	[216] 16.0
$\text{C}_3\text{H}_6\text{N}_4$	256.4	$A14 + 2*A15 + 3*A118 + A119 + A19 + 2*A1$ 2,5-dimethyltetrazole 13.5	0	52.65	13.5	[174] 11.8
$\text{C}_3\text{H}_6\text{N}_4\text{O}_4$	410	$A14 + 2*A15 + 3*A118 + A119 + A19 + 2*A1$ 1,3-dinitro-1,3-diazacyclopentane 25.1	0	62.3	25.1	[174] 27.1
		$A14 + 2*A15 + 2*A120 + 2*A51$				[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)	
$\text{C}_3\text{H}_6\text{N}_6\text{O}_3$	1,3,5-trinitroso-1,3,5-triazacyclohexane						
	367	17.78	48.45				
376	3.77	10.02	58.47	49.0	21.55	18.4	
$\text{C}_3\text{H}_6\text{N}_6\text{O}_5$	$A14 + 3*A15 + 3*A120 + 3*A52$						
	446	25.97	0	58.24	71.4	25.97	[216]
$\text{C}_3\text{H}_6\text{N}_6\text{O}_6$	1,3-dinitro-5-nitroso-1,3,5-triazacyclohexane						
	478.2	37.66	0	78.75	82.6	37.66	[225]
$\text{C}_3\text{H}_6\text{O}$	$A14 + A15*3 + 3*A120 + 3*A51$						
	176.6	5.72	0	32.34	39.7	5.72	[216]
$\text{C}_3\text{H}_6\text{O}$	acetone						
	161.3	6.57	0	40.75	37.5	6.57	[216]
$\text{C}_3\text{H}_6\text{O}$	propylene oxide						
	161.2	6.53	0	40.52	6.53	6.0	[216]
$\text{C}_3\text{H}_6\text{O}$	$A1 + A14 + A112 + A16$						
	171.3	8.59	0	50.14	46.3	8.59	[216]
$\text{C}_3\text{H}_6\text{O}_2$	propanal						
	252.7	10.66	0	42.2	38.1	10.66	[216]
$\text{C}_3\text{H}_6\text{O}_2$	$A1 + A2 + A34$						
	142.4	2.68	18.8	56.13	43.2	9.24	[216]
$\text{C}_3\text{H}_6\text{O}_2$	propionic acid						
	175.9	6.57	37.33	56.13	43.2	9.24	[216]
$\text{C}_3\text{H}_6\text{O}_2$	$A14 + 2*A15 + 2*A112$						
	174.9	7.49	0	42.82	42.8	7.49	[216]
$\text{C}_3\text{H}_6\text{O}_2\text{S}$	methyl acetate						
	291.9	16.97	0	58.15	53.4	16.97	[1]
$\text{C}_3\text{H}_7\text{O}_3$	β -thiolactic acid						
	289.9	11.34	0	39.12	42.2	11.34	[216]
$\text{C}_3\text{H}_6\text{O}_3$	$2*A2 + A36 + A86$						
	333.4	15.11	0	45.3	48.2	15.11	[216]
$\text{C}_3\text{H}_6\text{O}_3$	DL lactic acid						
	176.7	0.67	3.77	45.02	40.0	8.91	[216]
$\text{C}_3\text{H}_6\text{S}$	$A14 + 3*A15 + 3*A112$						
	199.9	8.24	41.25	45.02	40.0	8.91	[216]
$\text{C}_3\text{H}_7\text{Br}$	thiacyclobutane						
	184.1	6.53	0	35.5	43.1	6.53	[216]
$\text{C}_3\text{H}_7\text{Cl}$	$2*A1 + A3*B3 + A21$						
	156	7.39	0	47.37	36.3	7.39	[216]
$\text{C}_3\text{H}_7\text{N}$	2-chloropropane						
	237.8	13.18	0	55.44	40.0	13.18	[215]
$\text{C}_3\text{H}_7\text{NO}$	$A3*B3 + 2*A1 + A22$						
	212.9	8.95	0	42.05	42.1	8.95	[215]
$\text{C}_3\text{H}_7\text{NO}$	cyclopropylamine						
	303.8	9.73	0	32.01	36.6	9.73	[215]
$\text{C}_3\text{H}_7\text{NO}_2$	$2*A1 + A62$						
	321.9	15.23	0	47.31	52.6	15.23	[216]
$\text{C}_3\text{H}_7\text{NO}_2$	N,N-dimethylformamide						
	321.7	20.9	0	64.8	20.9	20.9	[216]
$\text{C}_3\text{H}_7\text{NO}_2$	N-methylacetamide						
	321.4	16.8	0	52.3	16.8	16.8	[270]
$\text{C}_3\text{H}_7\text{NO}_3$	$2*A1 + A60$						
	321.9	15.23	0	47.31	52.6	15.23	[216]
$\text{C}_3\text{H}_7\text{NO}_3$	ethyl carbamate						
	321.7	20.9	0	64.8	20.9	20.9	[216]
$\text{C}_3\text{H}_7\text{NO}_3$	$A1 + A2 + A70$						
	321.4	16.8	0	52.3	16.8	16.8	[215, 216]
$\text{C}_3\text{H}_7\text{NO}_3$	isopropyl nitrate						
	190.9	10.1	0	52.9	49.9	10.1	[216]
	$2*A1 + A3*B3 + A55$						
							[173]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C_3H_8	85.5	propane					
		3.52	0	41.24	42.3	3.52	3.6
$\text{C}_3\text{H}_8\text{N}_2\text{O}$	365.1 367.8	2*A1+A2					[215]
		N-ethylurea					
$\text{C}_3\text{H}_8\text{N}_2\text{O}$	454	14.39	0	39.41	47.2	14.39	17.2
		13.9	0	37.9		13.9	
$\text{C}_3\text{H}_8\text{N}_2\text{O}$	454	A1+A2+A67					[138]
		1,1-dimethylurea					
$\text{C}_3\text{H}_8\text{N}_2\text{O}$	379.5 301.2 161.3	2*A1+A65					[215]
		29.11	0	64.12	54.7	29.11	24.8
$\text{C}_3\text{H}_8\text{N}_2\text{O}$	379.5 301.2 161.3	1,3-dimethylurea					
		13	34.26				
$\text{C}_3\text{H}_8\text{O}$	148.8	0.08	0.26				
		0.32	1.97	36.48	36.6	13.4	5.91
$\text{C}_3\text{H}_8\text{O}$	148.8	2*A1+A66					[124, 138]
		1-propanol					
$\text{C}_3\text{H}_8\text{O}$	185.2 184.7	5.37	0	36.12	33.6	5.37	5.0
		A1+2*A2+A30					
$\text{C}_3\text{H}_8\text{O}_2$	168.0	2-propanol					
		5.41	0	29.21	27.3	5.41	5.1
$\text{C}_3\text{H}_8\text{O}_2$	168.0	5.37	0	29.1		5.37	
		2*A1+A3*B3+A30					
$\text{C}_3\text{H}_8\text{O}_3$	293 291	dimethoxymethane					
		8.33	0	49.59	51.7	8.33	8.7
$\text{C}_3\text{H}_8\text{O}_3$	293 291	2*A1+A2+2*A32					[216]
		1,2,3-trihydroxypropane					
$\text{C}_3\text{H}_8\text{S}$	167.2	18.28	0	62.34	55.6	18.28	16.3
		18.28	0	62.8		18.28	
$\text{C}_3\text{H}_8\text{S}$	167.2	2*A2+A3*B3+3*A30*C30					[215]
		ethyl methyl sulfide					
$\text{C}_3\text{H}_8\text{S}$	142.1 160	9.76	0	58.37	44.4	9.76	7.4
		2*A1+A2+A84					
$\text{C}_3\text{H}_8\text{S}$	142.1 160	1-propanethiol					
		3.97	27.95				
$\text{C}_3\text{H}_8\text{S}$	112.5 142.6	5.48	34.23	62.17	54.9	9.45	8.8
		A1+2*A2+A86					
$\text{C}_3\text{H}_8\text{SO}_2$	307.7	2-propanethiol					
		0.05	0.46				
$\text{C}_3\text{H}_9\text{Al}$	288.4	5.74	40.21	40.67	48.5	5.78	6.9
		2*A1+A3*B3+A86					
$\text{C}_3\text{H}_9\text{Al}$	288.4	ethylmethylsulfone					
		11.3	0	36.71	42.6	11.3	13.1
$\text{C}_3\text{H}_9\text{As}$	186.6	2*A1+A2+A88					[276]
		trimethylaluminum					
$\text{C}_3\text{H}_9\text{B}$	113.2	8.79	0	30.48	28.1	8.79	8.1
		3*A1+A97					
$\text{C}_3\text{H}_9\text{ClSi}$	185.1 218.0	trimethylarsine					
		8.96	0	48.03	46.3	8.96	8.6
$\text{C}_3\text{H}_9\text{Ga}$	257.9 244.5 257.8	3*A1+A98					[171]
		trimethylborane					
$\text{C}_3\text{H}_9\text{I}$	188.4 188.4	3.25	0	28.68	35.6	3.25	4.0
		3*A1+A99					
$\text{C}_3\text{H}_9\text{N}$	188.4 188.4	chlorotrimethylsilane					
		0.7	3.75				
$\text{C}_3\text{H}_9\text{N}$	178	9.68	44.42	48.17	41.8	10.38	9.1
		3*A1+A22*B22+A109					
$\text{C}_3\text{H}_9\text{N}$	188.4 188.4	trimethylgallium					
		11.05	0	42.83	40.8	11.05	10.5
$\text{C}_3\text{H}_9\text{N}$	188.4 188.4	0.33	1.4				
		10.6	41.1	42.5		11.0	
$\text{C}_3\text{H}_9\text{N}$	188.4 188.4	3*A1+A101					[216]
		1-aminopropane					
$\text{C}_3\text{H}_9\text{N}$	188.4 188.4	10.97	0	58.24	53.2	10.97	10.0
		10.63	0	56.4		10.63	
$\text{C}_3\text{H}_9\text{N}$	178	A1+2*A2+A45					[215, 216]
		2-aminopropane					
$\text{C}_3\text{H}_9\text{N}$	156.1	7.33	0	41.17	46.9	7.33	8.3
		2*A1+A3*B3+A45					
$\text{C}_3\text{H}_9\text{N}$	156.1	trimethylamine					
		6.54	0	41.92	30.5	6.54	4.8
		3*A1+A43					[215]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
$C_3H_{10}N_2$	222	1,2-diaminopropane 0.07	0.3			
	236.5	18.42	77.89	78.19	57.8	13.7 [50]
$C_3H_{10}N_2$	201.2	$A2 + A3 * B3 + A1 + 2 * A45$ trimethylhydrazine 9.49	0	47.13	25.2	9.49 [216]
		$3 * A1 + A44 * B44 + A43$ maleic anhydride 12.26	0	37.65	36.9	12.26 [216]
C_4H_3BrS	325.7	$A14 + 2 * A15 + 2 * A18 * B18 + A117$ 2-bromothiophene 0.01	0.25			
	55.3 205.3	7.9 $A14 + 2 * A15 + A21 + A131 + 2 * A18 + A18 * B18 + A19$ 2-chlorothiophene 8.97	38.43	38.7	42.7	7.91 [64]
C_4H_3ClS	201.3	$A14 + 2 * A15 + A22 * B22 + A131 + 2 * A18 + A18 * B18 + A19$ α -(trifluoromethoxy)- α , α -difluoromethyl acetate 8.51	0	50.84	52.0	8.51 [37]
	167.4	$3 * A25 + 2 * A26 + A1 + A38 + 2 * A4 * B4$ pyrazine 12.95	0	39.46	51.5	12.95 [216]
$C_4H_4N_2$		233.3	4 * $A10 + 2 * A41$ succinonitrile 6.2	26.57		
	331.2	3.7 $2 * A56 + 2 * A2$ N-nitro-bis(N,N-cyanomethyl) amine 38.66	11.21	37.78	49.7	9.9 [216]
$C_4H_4N_4O_2$	367	$2 * A2 + 2 * A56 * C56 + A51 * C51 + A47 * C47$ furan 2.05	13.64	105.34	94.9	38.66 [225]
	150.0 187.6	3.8 $A14 + 2 * A15 + A112 + 2 * A18 * B18 + 2 * A18$ 1,4-dioxane-2,5-dione 1.81	20.29	33.93	32.6	5.85 [216]
$C_4H_4O_4$	312.1	14.8 $3 * A15 + A14 + 2 * A115$ ethylene oxalate 13.4	5.82			
	356.2	14.8 $A14 + 3 * A15 + 2 * A115$ thiophene 1.21	41.55	47.36	50.8	16.61 [216]
C_4H_4S	415	13.4 $A14 + 2 * A15 + 2 * A18 * B18 + A131 + 2 * A18$ <i>cis</i> -3-chloro-2-butenic acid 13.81	0	32.29	50.8	13.4 [216]
	171.1 233.7 171.6 235.0	4.97 0.64 5.09 $A14 + 2 * A15 + 2 * A18 * B18 + A131 + 2 * A18$ <i>cis</i> -3-chloro-2-butenic acid 13.81	7.11 21.34 3.7 21.65	28.45	34.3	6.18 8.1 [216, 2]
$C_4H_5ClO_2$	333.7	$A36 * B36 + A1 + A7 + A6 * B6 + B22 * A22$ Z-3-chloro-2-butenic acid 20.71	0	41.42	43.1	13.81 [216]
	366.8	$A36 * B36 + A1 + A6 * B6 + A7 + A22 * B22$ E-3-chloro-2-butenic acid 13.81	0	56.48	43.09	20.71 [216]
$C_4H_5ClO_2$		333.7	$A36 * B36 + A1 + A6 * B6 + A7 + A22 * B22$ pyrrole 7.91	0	41.38	43.1
	C_4H_5N	249.7	$2 * A18 + A121 + A14 + 2 * A15 + 2 * A18 * B18$ succinimide 17.0	0	31.66	33.6
400		$A14 + 2 * A15 + A129$ 2-methylthiazole 12.16	43.44	42.5	42.2	17.0 [216]
	C_4H_5NS	248.6	$A14 + 2 * A15 + A131 + A118 + A1 + 2 * A18 * B18 + A19$ 4-methylthiazole 8.9	0	48.91	43.3
229.1		$A14 + 2 * A15 + A131 + A118 + A1 + 2 * A18 * B18 + A19$ 5-methylthiazole	0	38.85	43.3	8.9 [61]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
232.8	$A14+2*A15+A131+A118+A1+2*A18*B18+A19$	7.65	0	32.86	7.65	10.1
C_4H_6	1,3-butadiene					[61]
164.2	$2*A5+2*A6$	7.98	0	48.62	7.98	7.4
C_4H_6	1,2-butadiene					[215]
136.9	$A1+A5+A9+A6$	6.96	0	50.8	6.96	5.1
C_4H_6	2-butyne					[216]
240.9	$2*A1+2*A9$	9.25	0	38.38	9.25	7.1
C_4H_6	1-butyne					[215]
147.4	$A1+A2+A9+A8$	6.03	0	40.9	6.03	5.4
$C_4H_6N_6O_8$	1,3,5,5-tetranitro-1,3-diazacyclohexane					[216]
430	$A14+3*A15+2*A120+2*A51+2*A50+A17$	29.37	0	68.31	29.37	30.4
$C_4H_6O_2$	methyl acrylate					[225,193]
197.5	$A1+A5+A6*B6+A38$	9.73	0	49.26	9.73	9.2
$C_4H_6O_2$	α -methylacrylic acid					[216]
287.5	$A1+A36+A7+A5$	8.06	0	28.04	8.06	10.8
$C_4H_6O_2$	<i>cis</i> -crotonic acid					[216]
344.4	$A1+A6+A36+A6*B6$	12.57	0	36.49	12.57	13.8
$C_4H_6O_2$	γ -butyrolactone					[215]
230	$A14+2*A15+A115$	9.57	0	41.84	9.57	10.1
$C_4H_6O_3$	propylene carbonate					[32]
218.2	$2*A15+A14+A1+A16*B16+A116$	9.62	0	44.07	9.62	9.8
$C_4H_6O_4$	dimethyl oxalate					[89]
327.6	$2*A1+2*A38*B38$	21.07	0	64.32	21.07	16.5
$C_4H_6O_4$	succinic acid					[215]
457	$2*A36*B36+2*A2$	32.95	0	72.1	32.95	21.3
$C_4H_6O_5$	(<i>dl</i>) malic acid I					[340]
402	$A2+2*C36*A36+A3*B3+A30*C30$	33.52	0	83.39	33.52	30.0
$C_4H_6O_5$	(<i>dl</i>) malic acid II					[216]
396	$A2+2*C36*A36+A3*B3+A30*C30$	30.17	0	76.19	30.17	29.5
$C_4H_6O_5$	(<i>d</i>) malic acid					[216]
376	$A3*B3+2*C36*A36+A2+A30*C30$	23.01	0	61.2	23.01	28.0
C_4H_7NO	2-pyrrolidone					[273]
299	$A14+2*A15+A124$	13.92	0	46.56	13.92	13.0
C_4H_7NO	methacrylamide					[216]
385.1	$A1+A7+A5+A61$	15	0	38.95	15	20.1
C_4H_8	cyclobutane					[216]
145.7		5.71	39.17			
182.4	$A14+A15$	1.09	5.96	45.13	6.79	6.8
C_4H_8	1-butene					[216]
87.8	$A1+A2+A5+A6$	3.85	0	43.84	3.85	4.2
C_4H_8	<i>cis</i> -2-butene					[216]
134.3	$2*A1+2*A6$	7.31	0	54.43	7.31	6.1
C_4H_8	<i>trans</i> -2-butene					[216]
167.6	$2*A1+2*A6$	9.76	0	58.22	9.76	7.7
C_4H_8	isobutene					[216]
132.4		5.92	0	44.72	5.92	5.5

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_4H_8Br_2O_2$	$A7 + 2*A1 + A5$					[216]
363.2	(dl) 2,3-dibromo-1,4-butanediol 29.29	0	80.64	75.9	29.29	27.6
$C_4H_8Br_2O_2$	$2*A21 + 2*A2 + 2*A3*B3 + 2*A30*D30$					[226]
388.2	(d) 2,3-dibromo-1, 4-butanediol 33.89	0	87.3	75.9	33.89	29.5
$C_4H_8Cl_2O$	$2*A21 + 2*A2 + 2*A3*B3 + 2*A30*D30$					[226]
226.5	1,5-dichloro-3-oxapentane 8.39	0	37.02	65.6	8.39	14.9
$C_4H_8Cl_3O_4P$	$4*A2 + 2*A22*C22 + A32$					[216]
351.0	dimethyl (2,2,2-trichloro-1-hydroxyethyl)phosphonate 20.37	0	58.03	58.3	20.37	20.5
357	22.4	0	62.75	58.3	22.4	20.8
384	25	0	65.1	58.3	25.0	22.4
$C_4H_8N_2O_2$	$3*A22*E22 + A4*B4 + A3*B3 + A30*E30 + 2*A1 + A75$					[216]
408.2	N-acetylglycine amide 25.6	0	62.71	54.1	25.6	22.1
$C_4H_8N_4O_4$	$A1 + A2 + A61 + A60$					[216]
343	1,3-dinitro-1,3-diazacyclohexane 15.8	46.06				
354	2.97	8.39	54.45	69.9	18.77	24.7
$C_4H_8N_6O_5$	$A14 + 3*A15 + 2*A120 + 2*A51*C51$					[147]
404	1,5-dinitro-3-nitroso-1,3,5-triazacycloheptane 25.7	63.61				
440	2.9	6.59	70.2	75.1	28.6	33.1
$C_4H_8N_8O_8$	$A14 + 4*A15 + 3*A120 + 2*A51 + A52$					[147]
553.2	1,3,5,7-tetranitro-1,3,5,7-tetrazocine 69.87	0	126.3	102.7	69.87	56.8
$C_4H_8N_{12}O_6$	$A14 + 5*A15 + 4*A120 + 4*A51$					[216]
406	1,7-diazido-2,4,6-trinitro-2,4,6-triazazepentane 40.17	0	98.93	99.0	40.17	40.2
C_4H_8O	$4*A2 + 3*A51 + 2*A46 + 3*A47$					[225]
186.5	2-butanone 8.39	0	45.27	46.9	8.39	8.7
C_4H_8O	$2*A1 + A2 + A35$					[341]
176.8	butanal 11.09	61.09	62.8	53.5	11.09	9.4
C_4H_8O	$A1 + 2*A2 + A34$					[216, 84]
164.8	tetrahydrofuran 8.54	0	51.88	42.0	8.54	6.9
$C_4H_8O_2$	$A14 + 2*A15 + A112$					[215]
264.7	butanoic acid 11.07	0	41.82	45.2	11.07	12.0
$C_4H_8O_2$	$A1 + A2 + A36 + A2$					[215]
189.3	ethyl acetate 10.48	0	55.35	50.0	10.48	9.5
$C_4H_8O_2$	$2*A1 + A38 + A2$					[215]
272.9	1,4-dioxane 2.35	8.79				
284.1	12.84	45.19	53.97	46.9	15.2	13.3
$C_4H_8O_2S$	$A14 + 3*A15 + 2*A112$					[216]
288.6	tetramethylene sulfone 5.35	18.55				
301.6	1.43	4.73	23.29	30.4	6.78	9.2
$C_4H_8O_4$	$A14 + 2*A15 + A134$					[202]
385	tetroxane 22.6	0	58.58	56.8	22.6	21.9
C_4H_8S	$5*A15 + A14 + 4*A112$					[216]
177.0	thiacyclopentane 7.35	0	41.55	43.7	7.35	7.7
$C_4H_8S_2$	$A14 + 2*A15 + A131$					[136]
316.4	1,3-dithiane 0.8	2.53				
327.2	14.4	44.01	46.54	50.3	15.2	16.5
$C_4H_8S_2$	$A14 + 3*A15 + 2*A131$					[216]
384.6	1,4-dithiane 21.6	0	56.16	50.3	21.6	19.3

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_4\text{H}_9\text{Br}$	160.4	$A14 + 3*A15 + 2*A131$ 1-bromobutane 9.23	57.57	57.57	9.23	[216] 10.1
$\text{C}_4\text{H}_9\text{Br}$	208.6 231.5 256.1	$3*A2*B2 + A21 + A1$ <i>tert</i> -butyl bromide 5.65 1.05 1.97	27.08 4.52 7.68	39.33	8.66	[216] 12.2
$\text{C}_4\text{H}_9\text{Br}$	160.3	$3*A1 + A21 + A4*B4$ 2-bromobutane 6.88	0	42.92	6.88	[216] 8.0
$\text{C}_4\text{H}_9\text{Cl}$	182.9 219.3 248.1	$2*A1 + A2 + A3*B3 + A21$ <i>tert</i> -butyl chloride 1.87 5.88 1.97	10.25 26.82 7.95	45.02	9.82	[215] 10.1
$\text{C}_4\text{H}_9\text{N}$	207.1 215.3	$3*A1 + A4*B4 + A22$ pyrrolidine 0.54 8.58	2.61 39.84	42.44	9.12	[136] 9.3
$\text{C}_4\text{H}_9\text{NO}_2$	352.9 353.7 384.1	$A121 + A14 + 2*A15$ 2-amino-2-methylpropanediol 5 18.46 2.78	14.17 52.19 7.24	73.6	26.24	[216] 24.7
$\text{C}_4\text{H}_9\text{NO}_3$	310 361	$2*A2 + A4*B4 + 2*A30*C30 + A45 + A1$ 2-methyl-2-nitro-1-propanol 17.2 3.74	55.47 10.35	65.82	20.93	[274] 20.0
$\text{C}_4\text{H}_9\text{NO}_3$	352 424	$2*A1 + A4*B4 + A2 + A30*B30 + A50$ 2-methyl-2-nitro-1,3-propanediol 25.72 3.84	73.08 9.07	82.14	29.57	[216] 25.7
C_4H_{10}	107.6 134.9	$A1 + A4*B4 + 2*A2 + 2*A30*C30 + A50$ butane 2.07 4.66	19.06 34.56	53.62	6.73	[216] 6.7
C_4H_{10}	113.7	$2*A1 + 2*A2$ isobutane 4.54	0	40.11	4.54	[216] 4.1
$\text{C}_4\text{H}_{10}\text{Cl}_2\text{Si}$	174.1	$3*A1 + A3$ dichlorodiethylsilane 8.96	0	51.45	8.96	[216] 9.5
$\text{C}_4\text{H}_{10}\text{Hg}$	181.5	$2*A22*C22 + 2*A1 + 2*A2 + A109$ diethyl mercury 10.5	0	57.87	10.5	[216] 10.5
$\text{C}_4\text{H}_{10}\text{N}_2\text{O}$	381	$2*A1 + A104 + 2*A2$ N-propylurea 14.63	0	38.4	14.63	[216] 20.7
$\text{C}_4\text{H}_{10}\text{N}_2\text{O}$	429 375.5 280.8	$2*A2 + A1 + A67$ N-isopropylurea 17.5 2.31 1.41	40.79 6.15 5.02	51.97	21.22	[215] 13.5
$\text{C}_4\text{H}_{10}\text{N}_2\text{O}$	344.4	$2*A1 + A3*B3 + A67$ 1,1,3-trimethylurea 14.3	0	41.52	14.3	[138] 18.2
$\text{C}_4\text{H}_{10}\text{N}_4\text{O}_4$	410	$3*A1 + A64$ N-N'-dimethyl-N,N'-dinitro-1,2-ethanediamine 60.32	0	147.13	60.32	[215] 57.3
$\text{C}_4\text{H}_{10}\text{O}$	183.9	$2*A1 + 2*A2 + 2*A51 + 2*A47$ butyl alcohol 9.28	0	50.46	9.28	[225] 8.7
$\text{C}_4\text{H}_{10}\text{O}$	184.7	$3*A2*B2 + A1 + A30$ 2-butanol 5.97	0	32.33	5.97	[215] 6.4
$\text{C}_4\text{H}_{10}\text{O}$	286.1	$2*A1 + A2 + A3*B3 + A30$ <i>tert</i> -butyl alcohol 0.83	2.9			[76]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
294.5	0.49	1.66				
299.0	6.7	22.42	26.98	31.6	8.02	9.5
$C_4H_{10}O$	3*A1 + A4*B4 + A30 (+)2-butanol					[216]
	6	0	33.82	34.4	6	6.1
$C_4H_{10}O$	2*A1 + A2 + A3*B3 + A30 2-methyl-1-propanol					[76]
	6.32	0	36.93	27.7	6.32	4.7
$C_4H_{10}O$	2*A1 + A2 + A3 + A30 methyl isopropyl ether					[73]
	5.85	0	45.73	47.8	5.85	6.1
$C_4H_{10}O$	3*A1 + A32 + A3*B3 diethyl ether					[216]
	7.19	0	45.81	54.1	7.19	8.5
$C_4H_{10}O$	2*A1 + 2*A2 + A32 methyl propyl ether					[75]
	7.67	0	57.24	54.1	7.67	7.3
$C_4H_{10}O_2$	A32 + 2*A1 + 2*A2 1,4-dihydroxybutane					[216]
	18.7	0	63.7	73.6	18.7	21.6
$C_4H_{10}O_4$	4*A2*B2 + 2*A30*B30 1,2,3,4-tetrahydroxybutane					[216]
	42.36	0	106.97	86.6	42.36	34.3
$C_4H_{10}S$	2*A2 + 2*A3*B3 + 4*A30*D30 diethyl sulfide					[216]
	11.9	0	70.47	51.5	11.9	8.7
$C_4H_{10}S$	2*A1 + 2*A2 + A84 methyl propyl sulfide					[216]
	9.91	0	61.88	51.5	9.91	8.7
$C_4H_{10}S$	2*A1 + 2*A2 + A84 isopropyl methyl sulfide					[216]
	9.36	0	54.5	56.3	9.36	9.7
$C_4H_{10}S$	3*A1 + A3*B3 + A84 isobutyl mercaptan					[216]
	4.98	0	38.83	48.9	4.98	6.3
$C_4H_{10}S$	2*A1 + A3 + A2 + A86 <i>n</i> -butyl mercaptan					[216]
	10.46	0	66.44	68.6	10.46	10.8
$C_4H_{10}S$	A1 + 3*A2*B2 + A86 <i>tert</i> -butyl mercaptan					[216]
	4.07	26.83				
151.6	0.65	4.13				
157	0.97	4.87				
199.4	2.48	9.04	44.87	52.9	8.17	14.5
274.4						[216]
$C_4H_{10}S$	3*A1 + A4*B4 + A86 2-butanethiol					[216]
	6.48	0	48.7	55.5	6.48	7.4
$C_4H_{10}S_2$	2*A1 + A2 + A3*B3 + A86 diethyl disulfide					[216]
	9.4	0	54.77	59.0	9.4	10.1
$C_4H_{10}Zn$	2*A1 + 2*A2 + A85 diethyl zinc					[216]
	0.28	1.86				
148.4	16.63	70.19	72.05	60.5	17.52	14.3
237.0						[216, 96]
$C_4H_{11}N$	2*A1 + 2*A2 + A111 <i>tert</i> -butyl amine					[216, 96]
	0.11	1.24				
91.3	6.05	29.92				
202.3	0.88	4.28	35.44	51.3	7.05	4.7
206.2						[126]
$C_4H_{11}NO_2$	3*A1 + A4*B4 + A45 2-amino-2-methylpropane-1,3-diol					[126]
	25.21	71.61				
352	2.99	7.79	79.39	64.4	5.4	24.7
384						[216]
$C_4H_{11}NO_3$	2*A2 + A4*B4 + A1 + 2*A30*C30 + A45 2-amino-2-hydroxymethylpropane-1,3-diol					[216]
	2.41	5.43				
443.6	33.42	82.01	87.45	88.7	40.87	36.1
407.5						[34]
$C_4H_{12}Ge$	3*A2 + A4*B4 + 3*A30*D30 + A45 tetramethylgermanium					[34]
	7.45	0	40.4	35.1	7.45	6.5
184.4						[54]
	4*A1 + A102					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
$\text{C}_4\text{H}_{12}\text{N}_2$	1,2-diamino-2-methylpropane					
237.5	15.46	65.11				
256.1	2.23	8.71	73.81	62.2	13.03	15.9 [50]
$\text{C}_4\text{H}_{12}\text{Pb}$	2*A45+2*A1+A2+A4*B4 tetramethyllead					
242.9	10.8	0	44.45	40.2	10.8	9.8 [216]
$\text{C}_4\text{H}_{12}\text{Si}$	4*A1+A106 teramethylsilane					
174.0	6.74	0	38.73	43.2	6.74	7.5 [216]
$\text{C}_4\text{H}_{12}\text{Sn}$	4*A1+A109 tetramethyltin					
218.2	9.23	0	42.32	46.1	9.23	10.1 [166, 125]
$\text{C}_5\text{F}_{11}\text{N}$	4*A1+A110 perfluoropiperidine					
161	6.63	41.17				
171.9	1.84	10.71				
274.1	2.82	10.25	62.13	44.5	11.28	12.2 [216]
$\text{C}_5\text{F}_{13}\text{N}$	A14+3*A15+5*A17+A119+11*A28 perfluoromethyldiethylamine					
149.7	7.16	0	47.83	49.3	7.16	7.2 [216]
$\text{C}_5\text{H}_2\text{Cl}_3\text{O}$	4*A26+5*A4*B4+A43+9*A25 3,5,6-trichloro-2-pyridinol					
448.1	25.97	0	57.55	57.2	25.79	25.6 [215]
$\text{C}_5\text{H}_3\text{F}_7\text{O}_2$	3*A22*E22+A31+A41+A10+4*A12 methyl perfluorobutanoate					
191.4	11.7	0	61.49	62.3	11.77	11.8 [216]
$\text{C}_5\text{H}_4\text{O}_2$	A1+A38+4*A26+3*A25+3*A4*B4 furfural					
235.1	14.37	0	61.11	45.0	14.37	10.6 [216]
$\text{C}_5\text{H}_5\text{F}_3\text{O}_2$	A14+2*A15+2*A18+A18*B18+A19+A34+A112 trifluoromethyl (2-hydroxy-1-propenyl)ketone					
232.4	8.45	0	36.36	53.4	8.45	12.4 [216]
$\text{C}_5\text{H}_5\text{N}$	A4*B4+3*A25+A1+A6*B6+A7+A30*E30+A35 pyridine					
231.5	8.28	0	35.75	48.0	8.28	11.1 [216]
C_5H_6	5*A10+A41 cyclopentadiene					
176.6	8.01	0	45.36	34.3	8.01	6.1 [216]
$\text{C}_5\text{H}_6\text{N}_2$	A14+2*A15+4*A18 1,3-dicyanopropane					
244.2	12.59	0	51.55	63.5	12.59	15.5 [216]
$\text{C}_5\text{H}_6\text{N}_2$	2*A56+3*A2*B2 2,2-dicyanopropane					
302.6	9.87	32.59				
307.5	4.05	13.18	45.17	47.8	13.92	14.7 [216]
$\text{C}_5\text{H}_6\text{N}_2$	2*A56+A4*B4+2*A1 4-aminopyridine					
429.9	20.07	0	46.68	54.5	20.07	23.4 [221]
$\text{C}_5\text{H}_6\text{N}_2\text{O}_2$	4*A10+A12+A41+A45 thymine					
321.3	17.51	0	54.5	52.1	17.51	16.7 [216]
$\text{C}_5\text{H}_6\text{O}$	A14+3*A15+2*A124+A18*B18+A19+A1 2-methylfuran					
181.9	8.55	0	47.03	41.0	8.55	7.5 [106]
$\text{C}_5\text{H}_6\text{O}_2$	A1+A14+2*A15+2*A18+A19+A112+A18*B18 furfuryl alcohol					
258.6	13.1	0	50.75	48.7	13.1	12.6 [216]
$\text{C}_5\text{H}_6\text{S}$	A2+A14+2*A15+2*A18+A19+A112+A18*B18+A30*B30 2-methylthiophene					
207.8	9.47	0	45.57	42.7	9.47	8.9 [275]
$\text{C}_5\text{H}_6\text{S}$	A14+2*A15+A131+2*A18+A19+A1+A18*B18 3-methylthiophene					
204.2	10.54	0	51.62	41.2	10.54	8.4 [136]
$\text{C}_5\text{H}_7\text{N}$	A14+2*A15+A131+A1+A19+2*A18*B18+A18 N-methylpyrrole					
216.9	7.82	0	36.07	29.6	7.82	6.4 [216]
$\text{C}_5\text{H}_7\text{NO}_2$	A14+2*A15+A1+2*A18+2*A18*B18+A119 ethyl cyanoacetate					
246.8	11.78	0	47.73	57.3	11.78	14.1

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)	
C_5H_8	166.1	2*A2+A1+A38+A56 spiropentane 6.43	0	38.7	28.5	6.43	4.7
C_5H_8	132.4	2*A14+A17-A15 1-cis-3-pentadiene 5.64	0	42.61	50.7	5.64	6.7
C_5H_8	185.7	A1+A5+3*A6 trans-1,3-pentadiene 7.14	0	38.46	50.7	7.14	9.4
C_5H_8	124.3	A1+A5+3*A6 1,4-pentadiene 6.14	0	49.41	52.3	6.14	6.5
C_5H_8	127.3	A2+2*A5+2*A6 2-methyl-1,3-butadiene 4.92	0	38.68	34.7	4.92	4.4
C_5H_8	159.5	A1+A7+A5+2*A6 3-methyl-1,2-butadiene 7.95	0	49.84	39.0	7.95	6.2
C_5H_8	147.5	2*A1+A9+A5+A7 2,3-pentadiene 6.13	0	44.82	42.9	6.13	6.3
C_5H_8	135.9	2*A1+2*A6+A9 1,2-pentadiene 7.56	0	55.73	44.5	7.56	6.1
C_5H_8	87.07 138.1	A1+A2+A5+A6+A9 cyclopentene 0.48 3.36	5.51 24.32	29.83	37.6	3.84	5.2
C_5H_8	138.5	A14+2*A15+2*A18 methylenecyclobutane 5.86	0	42.31	42.2	5.86	5.8
$C_5H_8Br_4$	433.5	A14+A15+A5+A19 pentaerythryl tetrabromide 27.97	0	64.52	63.9	27.97	27.7
$C_5H_8Cl_2O$	292.2	4*A2+A4+4*A21 3,3-bis-(chloromethyl)oxacyclobutane 16.95	0	58	50.4	16.95	14.7
$C_5H_8F_4$	367.4 249.4	2*A2+2*A22*C22+A15+A14+A17+A112 pentaerythritol tetrafluoride 5.14 13.21	13.97 53.14	67.11	44.3	18.35	11.1
$C_5H_8O_2$	118 135 200 263	4*A2+4*A27+A4 δ -valerolactone 0.46 0.3 0.2 10.53	3.88 2.2 0.9 40.04	43.1	47.6	11.29	12.5
$C_5H_8O_2$	225	3*A15+A14+A115 methyl methacrylate 12.24	0	54.4	49.5	12.24	11.1
$C_5H_8O_2$	254.8	2*A1+A38+A7+A5 acetylacetone enol 14.5	0	56.91	66.0	14.5	16.8
$C_5H_8O_3$	306.2	2*A1+A35*B35+A30*B30+A6*B6+A7 levulinic acid 9.22	0	30.11	52.5	9.22	16.1
$C_5H_8O_4$	348.5 371	A1+2*A2+A35*B35+A36*B36 glutaric acid 2.46 20.9	7.07 56.33	63.4	60.2	23.36	22.3
C_5H_9Cl	169.4 180	3*A2*B2+2*A36*B36 chlorocyclopentane 7.63 0.64	45.05 3.54	48.59	36.8	8.27	6.6
C_5H_9N	213 232.7 292.1	A14+2*A15+A16+A22 2-cyano-2-methylpropane 0.23 1.91 9.29	1.09 7.78 31.8	40.67	47.6	11.43	13.9

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_5H_{10}ClNO$	351.3	3*A1+A4*B4+A56 2-chloro-N-isopropylacetamide 26.05	0	74.15	26.05	[216] 17.6
C_5H_9NO	342.3	2*A1+A2+A3*B3+A60+A22*B22 2-piperidone 16.1	0	47.02	16.1	[221] 16.2
C_5H_{10}	122 138 179.7	A14+3*A15+A124 cyclopentane 4.9 0.34 0.6	40.13 2.49 3.35	45.96	5.84	[227] 7.3 [216]
C_5H_{10}	121.8	A14+2*A15 <i>cis</i> -2-pentene 7.11	0	58.39	7.11	[215] 6.4
C_5H_{10}	133.0	2*A1+A2+2*A6 <i>trans</i> -2-pentene 8.35	0	62.82	8.35	[215] 7.0
C_5H_{10}	107.9	2*A1+A2+2*A6 1-pentene 5.81	55	53.82	5.81	[215] 5.9
C_5H_{10}	104.7	A1+2*A2+A5+A6 3-methyl-1-butene 5.36	0	51.19	5.36	[215] 4.3
C_5H_{10}	139.4	2*A1+A3+A5+A6 2-methyl-2-butene 7.60	0	54.47	7.60	[216] 8.3
C_5H_{10}	135.6	3*A1+A7+A5 2-methyl-1-butene 7.91	0	58.34	7.91	[216] 6.6
C_5H_{10}	138.6	2*A1+A2+A7+A5 methylcyclobutane 5.76	0	41.56	5.76	[216] 5.5
$C_5H_{10}N_2O_2$	431	A1+A14+A15+A16 N-acetyl-L-alanine amide 21.7	0	50.35	21.7	[215] 23.7
$C_5H_{10}N_2O_2S$	352.7	2*A1+A3*B3+A61+A60 5-methyl N-(methylcarbamoyloxy)thioacetimidate 21.73	0	61.61	21.73	[216] 18.7
$C_5H_{10}N_2O_3$	508.0	3*A1+A69+A42+A7+A84 alanylglycine (with decomp) 56.6	0	111.43	56.6	[221] 34.4
$C_5H_{10}N_4O_4$	369 374	A1+A2+A3*B3+A45+A36*C36+A60 1,3-dinitro-1,3-diazacycloheptane 21.8 2.8	59.08 7.49	66.57	24.6	[216] 27.5
$C_5H_{10}O$	158.5 183.9 272.1	A14+4*A15+2*A120+2*A51 pivaldehyde 0.5 4.81 2.52	3.15 26.15 9.26	38.56	7.83	[147] 14.0 [163]
$C_5H_{10}O$	118.5 180 234.2	3*A1+A4*B4+A34 3-pentanone 0.11 0.01 11.59	0.96 0.04 49.5	50.5	11.71	[341] 12.7 [341]
$C_5H_{10}O$	110 196.3	2*A1+2*A2+A35 2-pentanone 2.09 10.63	2.18 54.14	56.32	12.72	[341] 10.6
$C_5H_{10}O$	202.8 257.4	2*A1+2*A2+A35 cyclopentanol 3.71 1.54	18.28 5.98	24.27	5.24	[341] 7.2
$C_5H_{10}O$	180.0	A14+2*A15+A16+A30 isopropyl methyl ketone 9.34	0	51.9	9.34	[216] 8.5
$C_5H_{10}O_2$	239.5	3*A1+A3*B3+A35 pentanoic acid 14.16	0	59.14	14.16	[216] 14.1
		A1+3*A2*B2+A36				[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C ₅ H ₁₀ O ₂	278.3	2,2-dimethylpropanoic acid (pivalic acid)				
	309.1	8.18	29.39			
C ₅ H ₁₀ O ₄	426	2.27	7.34	36.74	43.3	10.45
	468	38.5	90.37	98.05	73.0	42.09
C ₅ H ₁₀ O ₅	334	21.9	0	65.6	65.4	21.9
		7.77	32.38			
C ₅ H ₁₀ S	172.4	8.87	0	51.48	46.5	8.87
		10.37	0	54	46.5	10.37
C ₅ H ₁₀ S	201.4	1.1	5.44			
	240.0	2.45	8.37	46.19	47.4	11.32
C ₅ H ₁₀ S	292.3	7.83	0	50.38	49.1	7.83
		14.37	77.61	77.61	72.5	14.37
C ₅ H ₁₁ Br	185.1	0.48	2.58			
		8.31	43.65	46.23	47.4	8.79
C ₅ H ₁₁ N	184.5	14.85	0	56.64	46.7	14.85
	190.4	18.8	0	41.1	41.1	18.8
C ₅ H ₁₁ NO	262.1	24.68	70.26			
		2.73	7.12	77.38	64.4	27.41
C ₅ H ₁₁ NO ₂	457.4	27.12	0	71.01	47.6	27.12
		3.26	12.69	31.1	35.5	5.83
C ₅ H ₁₁ NO ₂	351.3	20.49	0	63.85	51.7	20.49
	383.6	7.02	22.42			
C ₅ H ₁₁ NO ₃ S	382.0	0.88	2.55			
		14.55	39.4	64.37	68.1	22.45
C ₅ H ₁₂	143.5	8.4	0	58.58	63.2	8.4
		5.13	0	45.23	43.5	5.13
C ₅ H ₁₂	113.4	2.58	18.41			
		3.26	12.69	31.1	35.5	5.83
C ₅ H ₁₂	140	20.49	0	63.85	51.7	20.49
	256.5	7.02	22.42			
C ₅ H ₁₂ NO ₃ PS	321.0	0.88	2.55			
		14.55	39.4	64.37	68.1	22.45
C ₅ H ₁₂ N ₂ O	313.1	7.02	22.42			
	344.9	0.88	2.55			
C ₅ H ₁₂ N ₂ O	369.3	14.55	39.4	64.37	68.1	22.45
		0.1	0.41			
C ₅ H ₁₂ N ₂ O	249	33.13	73.65	74.06	52.4	33.23
	449.8	2.07	10.49			
C ₅ H ₁₂ N ₂ O	197.3	16.78	49.02	59.51	68.9	18.85
	342.3					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
C ₅ H ₁₂ N ₂ O	339.4	1,3-diethylurea 1.87	5.51			
	383.4	12.46	32.5	38.01	50.9	14.33
C ₅ H ₁₂ N ₂ O	272.2	2*A1 + A66 + 2*A2 tetramethylurea 13.4	0	49.23	51.0	13.4
		4*A1 + A63				13.9 [216]
C ₅ H ₁₂ N ₂ O ₂	331	N-methyl-N-nitrobutanamine 37.56	0	113.46	101.7	37.56
C ₅ H ₁₂ O	146 213 264	2*A1 + 3*A2 + A51 + A47 2,2-dimethyl-1-propanol 1.96	13.43			
		0.17				
		4.46	16.88	31.1	26.8	6.59
C ₅ H ₁₂ O	195.6	3*A1 + A4 + A2 + A30 1-pentanol 10.5	0	53.7	56.7	10.5
		A1 + 4*A2*B2 + A30				11.1 [216]
C ₅ H ₁₂ O	164.6	methyl <i>tert</i> -butyl ether 7.6	0	46.19	52.2	7.6
		4*A1 + A4*B4 + A32				8.6 [216]
C ₅ H ₁₂ O	145.7	ethyl propyl ether 8.39	0	57.61	61.3	8.39
		2*A1 + 3*A2 + A32				8.9 [216]
C ₅ H ₁₂ O	157.5	methyl <i>n</i> -butyl ether 10.85	0	68.9	61.3	10.85
		2*A1 + 3*A2 + A32				9.7 [216]
C ₅ H ₁₂ O ₂	248	1,5-pentanediol 15.72	0	63.6	82.9	15.72
		5*A2*B2 + 2*A30*B30				20.6 [216]
C ₅ H ₁₂ O ₂	146 213 264	2-methyl-2-butanol 1.96	13.44			
		0.17	0.78			
		4.46	16.88	31.1	38.8	6.59
C ₅ H ₁₂ O ₂	315.2 403.2	3*A1 + A4*B4 + A2 + A30 2,2-dimethyl-1,3-propanediol 13.8	43.78			
		4.6	11.41	55.19	50.8	18.4
C ₅ H ₁₂ O ₃	354 470	2*A1 + 2*A2 + A4 + 2*A30*B30 2-hydroxymethyl-2-methyl-1,3-propanediol 23.17	65.46			
		5.38	11.44	76.91	55.1	28.55
C ₅ H ₁₂ O ₄	460.4 538.7	A1 + 3*A2 + A4 + 3*A30*C30 pentaerythritol 43.93	95.4			
		7.11	13.2	108.78	85.4	51.04
C ₅ H ₁₂ O ₅	374.7	A4 + 4*A2 + 4*A30*D30 1,2,3,4,5-pentahydroxypentane (Ribitol) 37.6	0	100.35	90.4	37.6
		2*A2 + 3*A3*B3 + 5*A30*E30				39.9 [216]
C ₅ H ₁₂ O ₅	365.7	1,2,3,4,5-pentahydroxypentane (Xylitol) 37.4	0	102.27	90.4	37.4
		2*A2 + 3*A3*B3 + 5*A30*E30				33.1 [216]
C ₅ H ₁₂ O ₅	379.4	1,2,3,4,5-pentahydroxypentane (D-Arabitol) 38.9	0	102.53	90.4	38.9
		2*A2 + 3*A3*B3 + 5*A30*E30				34.3 [216]
C ₅ H ₁₂ S	190.8	methyl <i>tert</i> -butyl sulfide 8.41	0	44.1	49.6	8.41
		4*A1 + A4*B4 + A84				9.5 [216]
C ₅ H ₁₂ S	156.1	ethyl propyl sulfide 10.58	0	67.8	58.7	10.58
		2*A1 + 3*A2 + A84				9.2 [216]
C ₅ H ₁₂ S	175.6	methyl butyl sulfide 12.45	0	70.9	58.7	12.45
		2*A1 + 3*A2 + A84				10.3 [136]
C ₅ H ₁₂ S	139.6	3-methyl-1-butanethiol 7.41	0	53.05	56.1	7.41
		2*A1 + A3 + 2*A2 + A86				7.8 [216]
C ₅ H ₁₂ S	197.5	1-pentanethiol 17.53	0	88.78	77.9	17.53

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	$A1 + 4*A2*B2 + A86$					[216]
$C_5H_{12}S$	2-methyl-2-butanethiol					
144.5	7.06	48.87				
146.1	0.61	4.15	53.01	60.0	7.67	8.8
	$3*A1 + A4*B4 + A2 + A86$					[105]
$C_5H_{12}S$	3-methyl-2-butanethiol					
144.5	7.06	48.89				
146.1	0.61	4.16	53.05	49.7	7.67	7.3
	$3*A1 + A3 + A3*B3 + A86$					[216]
$C_5H_{12}SO_2$	<i>tert</i> -butylmethylsulfone					
357.6	24.69	0	69.03	47.7	24.69	17.1
	$4*A1 + A4*B4 + A88$					[276]
$C_5H_{12}S_4$	tetra(methylthia)methane					
296.4	6.11	20.5				
318.7	7.61	23.85				
338.7	4.14	12.13	56.48	55.9	14.78	18.9
	$4*A1 + A4*B4 + 4*A84$					[216]
$C_5H_{12}Si$	1,1-dimethyl-1-silacyclobutane					
155.5	6.76	42.87	43.48	37.6	6.76	5.8
	$A14 + A15 + A139 + 2*A1$					[153]
$C_5H_{12}Si$	vinyltrimethylsilane					
141.7	7.66	0	54.06	46.9	7.66	6.6
	$3*A1 + A5 + A6*B6 + A109$					[216]
$C_5H_{14}N_2$	N,N-dimethyl-1,3-propanediamine					
194.4	12.38	0	63.7	55.7	12.38	10.8
	$2*A1 + 3*A2 + A43 + A45$					[216]
C_6ClF_5	chloropentafluorobenzene					
191	3.64	19.04				
245	0.98	4.01				
257.5	8.36	32.45	55.5	54.5	12.36	14.0
	$5*A24 + A22*B22 + 6*A12$					[216]
$C_6Cl_3F_3$	1,3,5-trichloro-2,4,6-trifluorobenzene					
335.0	19.83	0	59.2	53.6	19.83	17.9
	$3*A22*D22 + 3*A24 + 6*A12$					[215]
$C_6Cl_4O_2$	2,3,5,6-tetrachloro-2,5-cyclohexadiene-1,4-dione					
567.2	30.87	0	54.43	57.4	30.87	32.6
	$A14 + 3*A15 + 2*A114 + 4*A19 + 4*A22*F22$					[215]
$C_6Cl_5NO_2$	pentachloronitrobenzene					
418	18.41	0	44.04	53.8	18.41	22.5
	$6*A12 + 5*F22*A22 + A50$					[215]
C_6Cl_6	hexachlorobenzene					
505	23.85	0	47.23	52.2	23.85	26.4
	$6*F22*A22 + 6*A12$					[215]
$C_6F_5NO_2$	pentafluoronitrobenzene					
250.5	11.81	0	47.13	56.0	11.81	14.0
	$5*A24 + A50 + 6*A12$					[216]
C_6F_6	hexafluorobenzene					
278.3	11.59	0	41.67	54.9	11.59	15.3
	$6*A24 + 6*A12$					[216]
C_6F_{14}	<i>n</i> -perfluorohexane					
103	0.97	10				
185	6.84	36.82	46.82	74.0	7.8	13.7
	$8*A26 + 6*A4*B4 + 6*A25$					[216, 67]
$C_6F_{15}N$	perfluorotriethylamine					
146.4	1.56	10.67				
156.2	5.56	35.61	46.28	59.1	7.12	9.2
	$6*A26 + A43 + 6*A4*B4 + 9*A25$					[216]
C_6N_4	tetracyanoethylene					
472.2	24.92	0	52.77	49.5	24.92	23.4
	$4*A56 + 2*A7$					[3]
C_6HBr_5O	pentabromophenol					
441.5	11.29	25.57				
502	19.14	38.13	63.7	63.1	30.43	31.7
	$6*A12 + A31 + 5*A21$					[191]
$C_6HCl_4NO_2$	1,2,4,5-tetrachloro-3-nitrobenzene					
373.3	19.46	0	52.13	52.5	19.46	19.6
	$4*E22*A22 + A50 + 5*A12 + A10$					[215]
C_6HCl_5	pentachlorobenzene					
357.7	20.6	0	57.59	50.9	20.6	18.2
	$5*A12 + 5*A22*E22 + A10$					[215]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
C ₆ HCl ₅ O	462.5	pentachlorophenol 17.15	0	37.08	17.15	26.0
		5*A22*F22+A31+6*A12				[215, 191]
C ₆ HF ₅	225.7	5*pentafluorobenzene 10.88	0	48.24	10.88	12.0
		5*A24+5*A12+A10				[215]
C ₆ HF ₅ O	287	5*pentafluorophenol 1.16	4.04			
	310.6	16.41	52.83	56.87	58.5	17.57
		6*A12+A31+5*A24				18.2
C ₆ H ₂ Br ₄	306.8	1,2,4,5-tetrabromobenzene 0.34	1.09			
	453.1	27.88	61.53	62.62	55.1	28.22
C ₆ H ₂ Cl ₄	320	4*1,2,3,4-tetrachlorobenzene 17	0	53.13	49.6	17
		4*A21+4*A12+2*A10				25.0
C ₆ H ₂ Cl ₄	421.2	1,2,4,5-tetrachlorobenzene 24.1	0	57.22	49.6	24.1
		4*A12+2*A10+4*A22*D22				20.9
C ₆ H ₂ Cl ₄	323.9	1,2,3,5-tetrachlorobenzene 19	0	58.66	49.6	19
		4*A12+2*A10+4*A22*D22				16.1
C ₆ H ₂ Cl ₅ N	505.8	pentachloroaniline 18.7	0	36.97	57.4	18.7
		6*A12+5*A22*F22+A45				29.0
C ₆ H ₂ F ₄	233.3	1,2,3,4-tetrafluorobenzene 10.93	0	46.85	51.4	10.93
		4*A12+2*A10+4*A24				12.0
C ₆ H ₂ F ₄	226.9	1,2,3,5-tetrafluorobenzene 10.67	0	47.01	51.4	10.67
		4*A12+2*A10+4*A24				11.7
C ₆ H ₂ F ₄	277	1,2,4,5-tetrafluorobenzene 15.05	0	54.31	51.4	15.05
		4*A12+2*A10+4*A24				14.3
C ₆ H ₂ F ₅ N	287.4	pentafluoroaniline 3.94	13.71			
	306.8	14.27	46.51	60.22	59.6	18.21
		5*A24+A45+6*A12				18.3
C ₆ H ₃ BrCl ₂ O	343.4	4-bromo-2,5-dichlorophenol 22.11	0	64.39	55.0	22.11
		2*A10+4*A12+2*A22*D22+A21+A31				18.9
C ₆ H ₃ Br ₃ O	366.2	2,4,6-tribromophenol 18.52	0	50.57	57.8	18.52
		4*A12+2*A10+3*A21+A31				21.2
C ₆ H ₃ Cl ₃	326.9	1,2,3-trichlorobenzene 20.5	0	62.71	48.4	20.5
		3*A10+3*A12+3*A22*C22				15.8
C ₆ H ₃ Cl ₃	336.7	1,3,5-trichlorobenzene 18.2	0	54.05	48.4	18.2
		3*A10+3*A12+3*A22*C22				16.3
C ₆ H ₃ Cl ₃ O	340.3	2,4,5-trichlorophenol 21.59	0	63.44	53.7	21.59
		4*A12+2*A10+3*A22*D22+A31				18.3
C ₆ H ₃ Cl ₄ N	337.2	2-chloro-6-(trichloromethyl)pyridine 20.3	0	60.2	58.0	20.3
		3*A10+A41+A11+A12+A4*B4+4*A22*E22				19.6
C ₆ H ₃ N ₃ O ₆	370	1,3,5-trinitrobenzene 1.9	5.13			
	380.3	14.8	38.95	44.08	53.0	16.71
		3*A10+3*A12+3*A50*C50				20.2
C ₆ H ₃ N ₃ O ₇	394.1	picric acid 17.1	0	43.39	58.4	17.1
		2*A10+4*A12+3*A50+A31				23.0
C ₆ H ₃ N ₃ O ₈	454.8	2,4,6-trinitroresorcinol 33.5	0	73.66	63.7	33.5
		A10+5*A12+2*A31+3*A50				29.0
C ₆ H ₄ BrCl		1,2-bromochlorobenzene				[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
260.6	12.37	0	47.47	48.4	12.37	12.6
$\text{C}_6\text{H}_4\text{BrCl}$	$A22*B22+A21+2*A12+4*A10$ 1,3-bromochlorobenzene					[216]
252.0	12.29	0	48.77	48.4	12.29	12.2
$\text{C}_6\text{H}_4\text{BrCl}$	$A22*B22+A21+2*A12+4*A10$ 1,4-bromochlorobenzene					[216]
337.8	18.76	0	55.54	48.4	18.76	16.4
$\text{C}_6\text{H}_4\text{BrI}$	$A22*B22+A21+2*A12+4*A10$ 1,2-bromiodobenzene					[216]
294.2	14.42	0	49.01	51.6	14.42	15.2
$\text{C}_6\text{H}_4\text{BrI}$	$4*A10+2*A12+A21+A29$ 1,3-bromiodobenzene					[215]
282.5	12.16	0	43.04	51.6	12.16	14.6
$\text{C}_6\text{H}_4\text{BrI}$	$4*A10+2*A12+A21+A29$ 1,4-bromiodobenzene					[215]
363.3	19.13	0	52.66	51.6	19.13	18.8
$\text{C}_6\text{H}_4\text{Br}_2$	$4*A10+2*A12+A21+A29$ 1,2-dibromobenzene					[215]
275	12.61	0	45.58	49.8	12.61	13.7
$\text{C}_6\text{H}_4\text{Br}_2$	$4*A10+2*A12+2*A21$ 1,3-dibromobenzene					[215]
266.3	13.21	0	49.61	49.8	13.21	13.3
$\text{C}_6\text{H}_4\text{Br}_2$	$4*A10+2*A12+2*A21$ 1,4-dibromobenzene					[215]
360.1	20.04	0	55.65	49.8	20.04	17.9
$\text{C}_6\text{H}_4\text{Br}_2\text{O}$	$2*A21+4*A10+2*A12$ 2,4-dibromophenol					[215]
313	14.64	0	46.79	55.2	14.64	17.3
$\text{C}_6\text{H}_4\text{ClNO}_2$	$3*A10+3*A12+2*A21+A31$ 1,2-chloronitrobenzene					[215]
308.2	19.08	0	61.9	48.6	19.08	15.0
$\text{C}_6\text{H}_4\text{ClNO}_2$	$4*A10+2*A12+A22*B22+A50$ 1,4-nitrochlorobenzene					[228]
354.6	11.85	0	33.42	48.6	11.85	17.2
$\text{C}_6\text{H}_4\text{ClNO}_2$	$4*A10+2*A12+A50+A22*B22$ 1,3-nitrochlorobenzene					[216]
317.6	19.37	0	60.99	48.6	19.37	15.4
$\text{C}_6\text{H}_4\text{Cl}_2$	$A22*B22+A50+4*A10+2*A12$ 1,2-dichlorobenzene					[215]
256.5	12.93	0	50.41	47.1	12.93	12.1
$\text{C}_6\text{H}_4\text{Cl}_2$	$4*A10+2*A12+2*A22*B22$ 1,3-dichlorobenzene					[215]
248.4	12.64	0	50.89	47.1	12.64	11.7
$\text{C}_6\text{H}_4\text{Cl}_2$	$4*A10+2*A12+2*A22*B22$ 1,4-dichlorobenzene					[215]
326	18.16	0	55.65	47.1	18.16	15.3
$\text{C}_6\text{H}_4\text{Cl}_2\text{N}_2\text{O}_2$	$2*A22*B22+4*A10+2*A12$ 2,6-dichloro-4-nitroaniline					[215]
466.8	32.64	0	69.92	56.4	32.64	26.3
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$	$4*A12+2*A10+A45+2*A22*D22+A50$ 2,3-dichlorophenol					[215]
330	21.36	0	64.73	52.4	21.36	17.3
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$	$3*A10+3*A12+A31+2*A22*C22$ 2,4-dichlorophenol					[215]
318	20.09	0	63.18	52.4	20.09	16.7
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$	$3*A10+3*A12+A31+2*A22*C22$ 2,5-dichlorophenol					[216]
331	22.43	0	67.76	52.4	22.43	17.4
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$	$3*A10+3*A12+A31+2*A22*C22$ 2,6-dichlorophenol					[216]
340	22.14	0	65.12	52.4	22.14	17.8
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$	$3*A10+3*A12+A31+2*A22*C22$ 3,4-dichlorophenol					[216]
341	20.93	0	61.38	52.4	20.93	17.9
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$	$3*A10+3*A12+A31+2*A22*C22$ 3,5-dichlorophenol					[216]
341	20.51	0	60.15	52.4	20.51	17.9
$\text{C}_6\text{H}_4\text{F}_2$	$3*A10+3*A12+A31+2*A22*C22$ 1,2-difluorobenzene					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
226	11.05	0	48.95	48.0	11.05	10.8
$\text{C}_6\text{H}_4\text{F}_2$	4*A10+2*A12+2*A24 1,3-difluorobenzene					[216]
186.8	0.83	4.43				
204.0	8.58	42.05	46.48	48.0	9.4	9.8
$\text{C}_6\text{H}_4\text{I}_2$	2*A24+2*A12+4*A10 1,2-diiodobenzene					[216]
296.6	14.01	0	47.24	53.5	14.01	15.9
$\text{C}_6\text{H}_4\text{I}_2$	2*A29+2*A12+4*A10 1,3-diiodobenzene					[215]
307.4	15.93	0	51.82	53.5	15.93	16.4
$\text{C}_6\text{H}_4\text{I}_2$	2*A29+2*A12+4*A10 1,4-diiodobenzene					[215]
402	22.37	0	55.65	53.5	22.37	21.5
$\text{C}_6\text{H}_4\text{N}_2\text{O}_4$	2*A29+2*A12+4*A10 1,2-dinitrobenzene					[215]
396.1	22.84	0	57.66	50.2	22.84	19.9
$\text{C}_6\text{H}_4\text{N}_2\text{O}_4$	4*A10+2*A12+2*A50 1,3-dinitrobenzene					[216]
363.2	17.36	0	47.82	50.2	17.36	18.2
$\text{C}_6\text{H}_4\text{N}_2\text{O}_4$	4*A10+2*A12+2*A50 1,4-dinitrobenzene					[215]
446.7	28.12	0	62.93	50.2	28.12	22.4
$\text{C}_6\text{H}_4\text{N}_2\text{O}_5$	4*A10+2*A12+2*A50 2,3-dinitrophenol					[215]
417	26.24	0	62.93	55.5	26.24	23.2
$\text{C}_6\text{H}_4\text{N}_2\text{O}_5$	3*A10+3*A12+2*A50+A31 2,4-dinitrophenol					[216]
388	24.17	0	62.29	55.5	24.17	21.6
$\text{C}_6\text{H}_4\text{N}_2\text{O}_5$	3*A10+3*A12+2*A50+A31 2,5-dinitrophenol					[216]
381	23.73	0	62.28	55.5	23.73	21.2
$\text{C}_6\text{H}_4\text{N}_2\text{O}_5$	3*A10+3*A12+2*A50+A31 2,6-dinitrophenol					[216]
336	19.58	0	58.27	55.5	19.58	18.7
$\text{C}_6\text{H}_4\text{N}_2\text{O}_5$	3*A10+3*A12+2*A50+A31 3,4-dinitrophenol					[216]
407	25.37	0	62.33	55.5	25.37	22.6
$\text{C}_6\text{H}_4\text{O}_2$	3*A10+3*A12+2*A50+A31 <i>p</i> -benzoquinone					[216]
388	18.45	0	47.56	29.4	18.45	11.4
$\text{C}_6\text{H}_5\text{Br}$	3*A15+A14+4*A18*B18+2*A114 bromobenzene					[215]
242.4	10.7	0	44.2	47.1	10.7	11.4
$\text{C}_6\text{H}_5\text{BrO}$	5*A10+A12+A21 4-bromophenol					[216]
336	16.57	0	49.32	52.5	16.57	17.6
$\text{C}_6\text{H}_5\text{Cl}$	A21+4*A10+2*A12+A31 chlorobenzene					[216]
227.9	9.55	0	41.92	40.4	9.55	9.2
$\text{C}_6\text{H}_5\text{ClO}$	5*A10+A22+A12 2-chlorophenol					[216]
276	0.09	0.33				
283	12.52	44.24	44.57	51.2	12.61	14.5
$\text{C}_6\text{H}_5\text{ClO}$	4*A10+2*A12+A22*B22+A31 3-chlorophenol					[215]
305.8	14.91	0	48.76	51.2	14.91	15.6
$\text{C}_6\text{H}_5\text{ClO}$	4*A10+2*A12+A22*B22+A31 4-chlorophenol					[215]
315.9	14.07	0	44.54	51.2	14.07	16.2
$\text{C}_6\text{H}_5\text{Cl}_2\text{N}$	4*A10+2*A12+A22*B22+A31 2,6-dichloro-4-benzenamine					[215]
467.2	29.48	0	63.11	53.5	29.48	25.0
$\text{C}_6\text{H}_5\text{Cl}_3\text{Si}$	3*A10+3*A12+2*A22*C22+A45 phenyltrichlorosilane					[221]
233.4	11.66	0	49.96	48.9	11.66	11.4
$\text{C}_6\text{H}_5\text{F}$	5*A10+A11+3*A22*D22+A109 fluorobenzene					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
230.9	11.31	0	48.95	46.2	11.31	10.7
$\text{C}_6\text{H}_5\text{I}$	5*A10+A12+A24 iodobenzene					[250]
241.8	9.75	0	40.31	49.0	9.75	11.8
$\text{C}_6\text{H}_5\text{NO}_2$	5*A10+A12+A29 picolinic acid					[216]
411	30	0	72.99	49.2	30	20.2
$\text{C}_6\text{H}_5\text{NO}_2$	4*A10+A12+A41+A36*B36 nicotinic acid					[216]
452	0.78	1.73				
510	26.7	52.35	54.08	49.2	27.48	25.1
$\text{C}_6\text{H}_5\text{NO}_2$	4*A10+A12+A41+A36*B36 isonicotinic acid					[182]
593	135	0	227.66	49.2	135	29.2
$\text{C}_6\text{H}_5\text{NO}_2$	4*A10+A12+A41+A36*B36 nitrobenzene					[216]
278.8	12.12	0	43.5	47.3	12.12	13.2
$\text{C}_6\text{H}_5\text{NO}_3$	5*A10+A12+A50 <i>o</i> -nitrophenol					[216]
318.2	17.45	0	54.83	52.7	17.45	16.8
$\text{C}_6\text{H}_5\text{NO}_3$	4*A10+2*A12+A50+A31 <i>m</i> -nitrophenol					[215,188]
371.2	19.19	0	51.7	52.7	19.19	19.6
$\text{C}_6\text{H}_5\text{NO}_3$	4*A10+2*A12+A50+A31 <i>p</i> -nitrophenol					[215,188]
388.2	18.25	0	47.02	52.7	18.25	20.5
C_6H_6	4*A10+2*A12+A50+A31 benzene					[216,188]
278.7	9.87	0	35.4	44.5	9.87	12.4
$\text{C}_6\text{H}_6\text{Cl}_6$	6*A10 1 α ,2 α ,3 β ,4 α ,5 α ,6 β -hexachlorocyclohexane					[216]
386.8	22.13	0	57.23	53.2	22.13	20.6
$\text{C}_6\text{H}_6\text{Cl}_6$	A14+3*A15+6*A16+6*A22*F22 1 α ,2 α ,3 β ,4 α ,5 α ,6 β -hexachlorocyclohexane (lindane)					[221]
388.9	15.9	0	40.88	53.2	15.9	20.7
$\text{C}_6\text{H}_6\text{N}_2\text{O}_2$	A14+3*A15+6*A16+6*A22*F22 2-nitroaniline					[221]
342.5	16.11	0	47.0	53.8	16.11	18.5
$\text{C}_6\text{H}_6\text{N}_2\text{O}_2$	4*A10+A45+A50+2*A12 3-nitroaniline					[216]
387	23.68	0	61.16	53.8	23.68	20.8
$\text{C}_6\text{H}_6\text{N}_2\text{O}_2$	4*A10+A45+A50+2*A12 4-nitroaniline					[216]
420.7	21.09	0	50.1	53.8	21.09	22.6
$\text{C}_6\text{H}_6\text{N}_6\text{O}_{14}$	4*A10+A45+A50+2*A12 2,2,2-trinitroethyl 4,4,4-trinitrobutyrate					[216]
362.7	25.94	71.52				
366.5	6.69	18.27	89.79	89.7	32.64	32.9
$\text{C}_6\text{H}_6\text{O}$	3*A2+2*A4*B4+A38+6*A50 phenol					[122]
314	11.51	0	36.82	49.9	11.51	15.7
$\text{C}_6\text{H}_6\text{O}_2$	5*A10+A31+A12 1,4-dihydroxybenzene					[216]
445	26.48	0	59.5	59.5	26.48	25.0
$\text{C}_6\text{H}_6\text{O}_2$	4*A10+2*A31+2*A12 1,2-dihydroxybenzene					[199]
376.9	22.01	0	58.39	55.2	22.01	20.8
$\text{C}_6\text{H}_6\text{O}_2$	4*A10+2*A31+2*A12 1,3-dihydroxybenzene					[199]
366.8	1.2	3.27				
382.6	18.9	49.41	52.64	55.2	20.1	21.1
$\text{C}_6\text{H}_6\text{O}_3$	4*A10+2*A31+2*A12 1,2,3-trihydroxybenzene					[199]
407.2	18.55	0	45.56	60.6	18.55	24.7
$\text{C}_6\text{H}_6\text{S}$	3*A10+3*A12+3*A31 thiophenol					[4]
258.3	11.4	0	44.3	52.6	11.3	13.6
$\text{C}_6\text{H}_7\text{N}$	5*A10+A12+A86 aniline					[281]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
267.1	10.54	0	39.45	51.0	10.54	14.1
$\text{C}_6\text{H}_7\text{N}$	5*A10+A12+A45 2-methylpyridine					[216]
206.5	9.72	0	47.1	48.5	9.72	10.0
$\text{C}_6\text{H}_7\text{N}$	4*A10+A11+A1+A41 3-methylpyridine					[216]
255	14.18	0	55.62	48.5	14.18	12.4
$\text{C}_6\text{H}_7\text{NO}$	4*A10+A11+A1+A41 <i>o</i> -aminophenol					[216]
447.4	34	0	75.99	56.3	34	25.2
$\text{C}_6\text{H}_7\text{NO}$	4*A10+2*A12+A31+A45 <i>m</i> -aminophenol					[216]
399	22.98	0	57.59	56.3	22.98	22.5
$\text{C}_6\text{H}_7\text{NO}$	4*A10+2*A12+A31+A45 <i>p</i> -aminophenol					[139]
459.5	31.2	0	67.9	56.3	31.2	25.9
462.5	26	0	56.22	56.3	26.0	26.0
C_6H_8	4*A10+2*A12+A31+A45 1,3-cyclohexadiene					[216,223]
161	4.2	0	26.1	38.0	4.2	6.1
C_6H_8	A14+3*A15+4*A18 1,4-cyclohexadiene					[216]
192	0.82	4.25				
224	5.72	25.51	29.76	38.0	6.53	8.5
$\text{C}_6\text{H}_8\text{N}_2$	A14+3*A15+4*A18 <i>o</i> -phenylenediamine					[216]
373.9	23.1	0	61.78	57.43	23.1	21.47
$\text{C}_6\text{H}_8\text{N}_2$	4*A10+2*A12+2*A45 <i>m</i> -phenylenediamine					[216]
335.5	15.4	0	45.9	57.43	15.4	19.27
$\text{C}_6\text{H}_8\text{N}_2$	4*A10+2*A12+2*A45 <i>p</i> -phenylenediamine					[216]
412.3	21.7	0	52.63	57.43	21.7	23.68
$\text{C}_6\text{H}_8\text{N}_2$	4*A10+2*A12+2*A45 phenylhydrazine					[216]
292.8	16.43	0	56.11	45.7	16.43	13.4
$\text{C}_6\text{H}_8\text{N}_2\text{O}_2$	5*A10+A12+A45+A44 N-acetylglycine amide					[215]
408.2	25.6	0	62.71	54.1	25.6	22.1
$\text{C}_6\text{H}_8\text{N}_2\text{O}_2$	A1+A60+A2+A61 1,3-dimethyluracil					[278]
398	14.6	0	36.68	30.0	14.6	11.9
$\text{C}_6\text{H}_8\text{N}_4\text{O}_2$	2*A1+A14+3*A15+2*A125+2*A18*B18 <i>bis</i> (2-cyanoethyl)-N-nitroamine					[292]
327	44.99	0	137.57	109.1	44.99	35.7
$\text{C}_6\text{H}_8\text{O}_2$	4*A2+2*A56+A51+A47 1,4-cyclohexanedione					[225]
322.2	6.15	19.09				
339.2	0.96	2.83				
348.2	10.04	28.84	50.76	41.8	17.15	14.5
$\text{C}_6\text{H}_8\text{O}_4$	3*A15+A14+2*A114 dimethyl maleate					[114]
254	14.64	0	57.74	58.4	14.64	14.8
$\text{C}_6\text{H}_8\text{O}_4$	2*A1+2*B6*A6+2*A38 dimethyl fumarate					[216]
375	35.15	0	93.72	58.4	35.15	21.9
$\text{C}_6\text{H}_8\text{O}_4$	2*A1+2*A38+2*B6*A6 DL 3,6-dimethyl-1,4-dioxane-2,5-dione					[216]
397.5	24.7	0	62.14	49.1	24.7	19.5
$\text{C}_6\text{H}_8\text{S}$	A14+A15+2*A115+2*A16+2*A1 2,5-dimethylthiophene					[216]
210.6	8.91	0	42.31	51.1	8.91	10.8
$\text{C}_6\text{H}_8\text{ClO}_2$	2*A1+A131+A14+2*A15+2*A19+2*A18 chloroethyl methacrylate					[216]
235.1	17	0	72.31	62.3	17	14.7
$\text{C}_6\text{H}_9\text{N}$	2*A2+A22*B22+A5+A7+A1+A38 2,4-dimethylpyrrole					[216]
268.5	9.6	0	35.75	48.9	9.6	13.1

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_6\text{H}_9\text{N}$	280.9	A 14+2*A 15+A 18+2*A 1+A 121+A 18*B 18+2*A 19 2,5-dimethylpyrrole		33.09	9.3	[70]
$\text{C}_6\text{H}_9\text{NS}$	240.7	A 14+2*A 15+2*A 18+2*A 1+A 121+2*A 19 2,4,5-trimethylthiazole		37.39	9	[216]
C_6H_{10}	138.7 169.7	A 14+2*A 15+3*A 19+3*A 1+A 118+A 131 cyclohexane		49.85	7.51	[61]
$\text{C}_6\text{H}_{10}\text{N}_2\text{O}$	359.3 399.3 438	A 14+3*A 15+2*A 18 2,3-diazabicyclo[2.2.2]oct-2-ene N-oxide		42.9	16.91	[216]
$\text{C}_6\text{H}_{10}\text{O}$	220.8 245.2	2*A 14+2*A 15+2*A 16+A 123 cyclohexanone		44.64	9.99	[42]
$\text{C}_6\text{H}_{10}\text{O}$	193.1 238.1	A 14+3*A 15+A 114 cyclohexene oxide		53.85	10.6	[156]
$\text{C}_6\text{H}_{10}\text{O}_2$	272	2*A 14+A 15+A 112+2*A 16 ϵ -caprolactone		50.79	13.82	[32]
$\text{C}_6\text{H}_{10}\text{O}_3$	324.1 387.2	A 14+4*A 15+A 115 2,2-dimethyltrimethylene carbonate		46.31	15.92	[200]
$\text{C}_6\text{H}_{10}\text{O}_4$	426.4	A 14+3*A 15+A 116+2*A 1+A 17 adipic acid		81.73	34.85	[340]
$\text{C}_6\text{H}_{10}\text{O}_6$	360.2	4*A 2*B 2+2*A 36*B 36 (dl) dimethyl tartrate		74.81	26.94	[220]
$\text{C}_6\text{H}_{10}\text{O}_6$	322.2	2*A 38+2*A 3*B 3+2*A 1+2*A 30*D 30 (d) dimethyl tartrate		53.89	17.36	[220]
$\text{C}_6\text{H}_{11}\text{Br}$	216.9	2*A 38+2*A 3*B 3+2*A 1+2*A 30*D 30 bromocyclohexane		49.75	10.79	[190]
$\text{C}_6\text{H}_{11}\text{Cl}$	120 220.4 229.3	A 14+3*A 15+A 21+A 16 chlorocyclohexane		45.67	10.1	[229]
$\text{C}_6\text{H}_{11}\text{NO}$	240.8 362.6 273.4	A 14+3*A 15+A 16+A 22 cyclohexanone oxime		35.43	12.81	[5]
$\text{C}_6\text{H}_{11}\text{NO}$	343.3	A 14+3*A 15+A 19+A 53 ϵ -caprolactam		46.89	16.1	[6]
$\text{C}_6\text{H}_{11}\text{NO}_3$	431.4	A 14+4*A 15+A 124 N-dimethylaminosuccinamic acid		85.71	36.97	[221]
$\text{C}_6\text{H}_{11}\text{N}_2\text{O}_3\text{PS}_2$	315.1	2*A 1+2*A 2+A 36*B 36+A 59 S-2,3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl O,O-dimethyl phosphorodithioate		90.59	28.54	[221]
C_6H_{12}	186.1 279.8	3*A 1+A 14+2*A 15+A 138+A 19+A 118+A 32+A 80 cyclohexane		45.77	9.41	[216]
C_6H_{12}	130.7	A 14+3*A 15 methylcyclopentane		53.01	6.93	[216]
		A 14+A 16+A 1+2*A 15				[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C_6H_{12}	133.4	1-hexene 9.35	0	70.1	61.6	9.37
		$A1 + 3*A2 + A5 + A6$				8.2 [216]
C_6H_{12}	196.8	2,3-dimethyl-2-butene 3.53	17.94			
	198.9	6.44	32.39	50.34	48.9	9.97
		$4*A1 + 2*A7$				9.6 [216]
C_6H_{12}	124.9	3,3-dimethyl-1-butene 4.35	34.84			
	158.4	1.09	6.87	41.71	40.5	5.44
		$A4 + 3*A1 + A5 + A6$				5.1 [216]
C_6H_{12}	132	<i>cis</i> -2-hexene 8.88	0	67.27	59.9	8.88
		$2*A1 + 2*A2 + 2*A6$				7.9 [165]
$\text{C}_6\text{H}_{12}\text{N}_2$	351.1	1,4-diazabicyclo[2.2.2]octane 10.54	30.08			
	433	7.45	17.15	47.24	35.6	18.0
		$2*A14 + 2*A15 + 2*A119$				15.4 [216]
$\text{C}_6\text{H}_{12}\text{N}_2\text{O}_3$	480.1	β -alanyl- β -alanine 58.3	0	121.45	81.4	58.3
		$4*A2 + A45 + A36*C36 + A60$				39.1 [216]
$\text{C}_6\text{H}_{12}\text{N}_2\text{O}_3$	483.2	α -alanyl- α -alanine (DL) 33.2	0	68.72	68.4	33.2
		$2*A1 + A45 + A36*C36 + A60 + 2*A3*B3$				33.0 [216]
$\text{C}_6\text{H}_{12}\text{O}$	265.5	cyclohexanol 8.8	33.3			
	299.1	1.8	6.0	39.3	31.5	9.9
		$A14 + 3*A15 + A16 + A30$				9.4 [81]
$\text{C}_6\text{H}_{12}\text{O}$	310.2	1-methylcyclopentanol 8.41	0	27.11	25.5	8.41
		$A14 + 2*A15 + A1 + A17 + A30$				7.9 [230]
$\text{C}_6\text{H}_{12}\text{O}$	214.9	hexanal 13.3	61.89			
	243.2	0.34	1.38	63.27	76.4	13.64
		$A14 + 4*A2*B2 + A34$				18.6 [128, 168]
$\text{C}_6\text{H}_{12}\text{O}$	221.7	3,3-dimethyl-2-butanone 11.34	0	51.04	52.0	11.34
		$4*A1 + A4*B4 + A35$				11.5 [216]
$\text{C}_6\text{H}_{12}\text{O}$	145	3-hexanone 0.68	4.7			
	217.7	13.47	61.89	66.61	61.1	14.15
		$2*A1 + 3*A2 + A35$				13.3 [216]
$\text{C}_6\text{H}_{12}\text{O}$	217.7	2-hexanone 14.9	68.42	68.41	61.1	14.9
		$2*A1 + 3*A2 + A35$				13.3 [216]
$\text{C}_6\text{H}_{12}\text{O}_2$	229.6	2,2-dimethyl-1,3-dioxane 12.1	0	52.7	47.5	12.1
		$A14 + 3*A15 + 2*A1 + A17 + 2*A112$				10.9 [47]
$\text{C}_6\text{H}_{12}\text{O}_2$	360.4	<i>cis</i> -1,2-cyclohexanediol 19.89	55.19			
	371.6	3.32	8.93	64.12	51.2	23.21
		$A14 + 3*A15 + 2*A30*B30 + 2*A16$				19.0 [204]
$\text{C}_6\text{H}_{12}\text{O}_2$	372.3	<i>trans</i> -1,2-cyclohexanediol 18.51	0	49.72	51.2	18.51
		$A14 + 3*A15 + 2*A30*B30 + 2*A16$				19.1 [204]
$\text{C}_6\text{H}_{12}\text{O}_3$	142.7	2,4,6-trimethyl-1,3,5-trioxane 0.26	1.81			
	147.5	0.77	5.24			
	285.7	13.52	47.32	54.37	56.7	14.55
		$3*A1 + 3*A16 + A14 + 3*A15 + 3*A112$				16.2 [216]
$\text{C}_6\text{H}_{12}\text{O}_6$	414	α -D-glucose 31.42	0	75.9	93.0	31.42
		$A14 + 3*A15 + 5*A30*F30 + A2 + 5*A16 + A112$				38.5 [216]
$\text{C}_6\text{H}_{12}\text{O}_6$	496.9	myo-inositol 47.9	0	96.4	92.7	47.9
		$A14 + 3*A15 + 6*A16 + 6*A30*F30$				46.1 [216]
$\text{C}_6\text{H}_{12}\text{S}$	165	cyclopentyl methyl sulfide 0.9	5.44			
	169.9	9.2	54.31	59.75	45.7	10.1
		$A14 + 2*A15 + A1 + A84 + A16$				7.8 [105]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_6\text{H}_{12}\text{S}$	189.6	cyclohexanethiol 10	0	52.72	10.0	10.0
		$A14+3*A15+A86+A16$				[341]
$\text{C}_6\text{H}_{13}\text{Br}$	188.1	1-bromohexane 18.05	0	95.98	18.05	15.4
		$A1+5*A2*B2+A21$				[216]
$\text{C}_6\text{H}_{13}\text{N}$	269.4	2-methylpiperidine 18.58	0	68.99	18.58	13.3
		$A14+3*A15+A121+A1+A16$				[216]
$\text{C}_6\text{H}_{13}\text{NO}$	374	hexanamide 25.1	0	67.12	25.1	31.0
		$4*A2*B2+A1+A61$				[279]
C_6H_{14}	177.8	<i>n</i> -hexane 13.08	0	73.22	13.08	12.9
		$2*A1+4*A2*B2$				[216]
C_6H_{14}	136.1	2,3-dimethylbutane 6.43	47.22			
	107	2.37	22.13			
	145.2	0.79	5.47	52.96	37.6	5.1
		$4*A1+2*A3$			9.59	[216]
C_6H_{14}	110.3	3-methylpentane 5.31	0	48.17	5.31	5.6
		$2*A2+3*A1+A3$				[216]
C_6H_{14}	119.6	2-methylpentane 6.27	0	52.43	6.27	6.05
		$2*A2+3*A1+A3$				[216]
C_6H_{14}	126.8	2,2-dimethylbutane 5.4	42.57			
	140.8	0.28	2.02			
	174.3	0.58	3.31	45.88	42.6	7.4
		$4*A1+A2+A4$			6.26	[216]
$\text{C}_6\text{H}_{14}\text{O}$	225.8	1-hexanol 15.48	0	68.56	15.48	14.9
		$A1+5*A2*B2+A30$				[216]
$\text{C}_6\text{H}_{14}\text{O}$	187.8	isopropyl ether 12.05	0	64.02	12.05	10.5
		$4*A1+2*A3*B3+A32$				[66]
$\text{C}_6\text{H}_{14}\text{O}$	158.4	4-oxaheptane 10.77	0	67.99	10.77	10.8
		$2*A1+4*A2+A32$				[216]
$\text{C}_6\text{H}_{14}\text{O}_2$	316.2	2,3-dimethyl-2,3-butanediol 14.7	0	46.49	14.7	19.2
		$4*A1+2*A4*B4+2*B30*A30$				[231]
$\text{C}_6\text{H}_{14}\text{O}_2$	320.6	1,6-hexanediol 25.52	0	79.6	25.52	29.0
		$2*A30*B30+6*A2*B2$				[216]
$\text{C}_6\text{H}_{14}\text{O}_3$	209.1	2,5,8-trioxanonane 17.8	0	85.1	17.8	16.3
		$2*A1+4*A2+3*A32$				[216]
$\text{C}_6\text{H}_{14}\text{O}_6$	366.5	D sorbitol 30.2	0	82.4	30.2	40.9
		$2*A2+4*A3*B3+6*A30*F30$				[216]
$\text{C}_6\text{H}_{14}\text{O}_6$	460.3	dulcitol 65.1	0	141.4	65.1	51.4
		$2*A2+4*A3*B3+6*A30*F30$				[216]
$\text{C}_6\text{H}_{14}\text{O}_6$	439.1	D mannitol 56.1	0	127.8	56.1	49.0
	438.7	50.6	0	115.3	50.6	49.0
		$2*A2+4*A3*B3+6*A30*F30$				[216, 394]
$\text{C}_6\text{H}_{14}\text{S}$	195.1	diisopropyl sulfide 10.42	0	53.39	10.42	10.4
		$4*A1+2*A3*B3+A84$				[341]
$\text{C}_6\text{H}_{14}\text{S}$	170.4	dipropyl sulfide 12.14	0	71.25	12.14	11.2
		$2*A1+4*A2+A84$				[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$C_6H_{14}S$	butyl ethyl sulfide					
178.1	12.39	0	69.57	65.8	12.39	11.7
	$2*A1 + 4*A2 + A84$					[136]
$C_6H_{14}S$	1-hexanethiol					
192.6	18.03	0	93.51	87.2	18.03	16.8
	$5*A2*B2 + A1 + A86$					[216]
$C_6H_{14}S_2$	dipropyl disulfide					
187.7	13.81	0	73.55	73.3	13.81	13.8
	$2*A1 + 4*A2 + A85$					[216]
$C_6H_{15}Al$	triethylaluminum					
225	10.6	0	47.11	49.5	10.6	11.1
	$3*A1 + 3*A2 + A97$					[216]
$C_6H_{15}As$	triethylarsine					
181.8	11.06	0	60.83	67.7	11.06	12.3
	$3*A1 + 3*A2 + A98$					[216]
$C_6H_{15}B$	triethylborane					
180.3	11.85	0	65.7	57.0	11.85	10.3
	$3*A1 + 3*A2 + A99$					[216]
$C_6H_{15}Bi$	triethylbismuth					
145.8	8.7	0	59.64	59.7	8.7	8.7
	$3*A1 + 3*A2 + A100$					[167]
$C_6H_{15}Ga$	triethylgallium					
193.5	11.64	0	60.18	62.2	11.64	12.0
	$3*A1 + 3*A2 + A101$					[216]
$C_6H_{15}In$	triethylindium					
237.6	13.01	0	54.76	54.8	13.01	13.0
	$3*A1 + 3*A2 + A105$					[216]
$C_6H_{15}Sb$	triethylantimony					
153.9	9.45	0	61.42	61.4	9.45	9.5
	$3*A1 + 3*A2 + A107$					[216]
$C_6H_{16}Si_2$	1,1,3,3-tetramethyl-1,3-disilacyclobutane					
266	10.26	0	38.57	38.0	10.26	10.1
	$A14 + A15 + 2*A139 + 4*A1$					[216]
$C_6H_{18}OSi_2$	hexamethyldisiloxane					
204.9	11.92	0	58.17	56.0	11.92	11.5
	$6*A1 + A32*B32 + 2*A109$					[216]
$C_6H_{18}O_3Si_3$	hexamethylcyclotrisiloxane					
335.2	16.61	0	49.55	49.6	16.61	16.6
	$A14 + 3*A15 + 6*A1 + 3*A112 + 3*A139$					[216,121]
$C_6H_{18}Si_2$	hexamethyldisilane					
221.8	9.75	43.95				
287.7	3.02	10.49	54.44	51.3	12.77	14.8
	$6*A1 + 2*A109$					[216]
$C_6H_{21}N_3Si_3$	hexamethylcyclotrisilazane					
254.4	15.17	0	59.63	52.4	15.17	13.3
	$A14 + 3*A15 + 3*A139 + 6*A1 + 3*A121$					[216]
C_7F_8	perfluorotoluene					
207	11.49	0	55.23	53.0	11.49	11.0
	$5*A12 + A11 + A4*B4 + 5*A24 + 3*A25$					[216]
C_7F_{16}	perfluoroheptane					
180.4	6.67	36.97				
221.9	6.95	31.31	68.28	83.1	13.62	18.5
	$7*A4*B4 + 6*A25 + 10*A26$					[216,67]
$C_7H_3Br_2NO$	3,5-dibromo-4-hydroxybenzonitrile					
464	32.03	0	69.03	58.0	32.03	26.9
	$2*A21 + A56 + A31 + 4*A12 + 2*A10$					[221]
$C_7H_3F_5$	2,3,4,5,6-pentafluorotoluene					
243.7	13.28	0	54.48	53.7	13.28	13.1
	$5*A12 + A11 + A1 + 5*A24$					[216,77]
$C_7H_3Cl_2N$	2,6-dichlorobenzonitrile					
417.2	26.17	0	62.73	49.9	26.17	20.8
	$2*A22*C22 + A56 + 3*A12 + 3*A10$					[215]
$C_7H_3Cl_3O_2$	2,3,6-trichlorobenzoic acid					
402.7	23.85	0	59.23	63.5	23.85	25.6
	$4*A12 + 2*A10 + 3*A22*D22 + A36*D36$					[215]
$C_7H_3I_2NO$	4-hydroxy-3,5-diiodobenzonitrile					
482.9	33.63	0	69.64	61.7	33.63	29.8
	$4*A12 + 2*A10 + 2*A29 + A56 + A31$					[221]
$C_7H_3I_3O_2$	2,3,5-triiodobenzoic acid					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
503.8	32.23	0	63.97	73.1	32.23	36.8
$C_7H_4Cl_2O_2$	3*A29+A36*D36+4*A12+2*A10 3,5-dichlorobenzoic acid					[215]
459.3	22.97	0	50.01	62.2	22.97	28.6
$C_7H_4Cl_3NO_3$	3*A12+3*A10+2*A22*C22+A36*C36 3,5,6-trichloro-2-pyridinyloxyacetic acid					[215]
423.3	31.17	0	73.63	78.8	31.17	33.4
$C_7H_4N_2O_6$	A10+4*A12+3*A22*F22+A41+A32+A36*F36+A2 3,5-dinitrobenzoic acid					[221]
480.4	22.8	0	47.47	65.3	22.8	31.4
$C_7H_5Cl_3N_2O_2$	3*A12+2*A50+A36*C36+3*A10 methyl 4-amino-3,5,6-trichloro-2-picolinate					[280]
394.3	26.78	0	67.91	68.7	26.78	27.1
$C_7H_5ClO_2$	5*A12+A41+A38+3*A22*F22+A45+A1 2-chlorobenzoic acid					[232]
413.4	25.73	0	62.34	47.0	25.73	19.4
$C_7H_5ClO_2$	4*A10+A36*B36+2*A12+A22*B22 3-chlorobenzoic acid					[215]
427.4	23.85	0	55.65	47.0	23.85	20.1
$C_7H_5ClO_2$	4*A10+A36*B36+2*A12+A22*B22 4-chlorobenzoic acid					[215]
512.9	32.26	0	62.76	47.0	32.26	24.1
$C_7H_5Cl_2NO_2$	4*A10+A36*B36+2*A12+A22*B22 3-amino-2,5-dichlorobenzoic acid					[215]
475.6	37.42	0	78.68	68.7	37.42	32.7
$C_7H_5Cl_3$	2*A22*D22+A45+A36*D36+4*A12+2*A10 benzotrichloride					[215]
236.0	13.95	0	59.11	53.2	13.95	12.6
$C_7H_5F_3$	5*A10+A11+3*A22*C22+A4*B4 benzotrifluoride					[216]
244.1	13.78	0	56.45	44.7	13.77	10.9
$C_7H_5IO_2$	5*A10+A11+A4*B4+3*A25 2-iodobenzoic acid					[216]
435.1	21.38	0	49.14	50.2	21.38	21.8
$C_7H_5IO_2$	4*A10+2*A12+A36*B36+A29 3-iodobenzoic acid					[7]
460.4	28.7	0	62.34	50.2	28.7	23.1
$C_7H_5IO_2$	4*A10+2*A12+A36*B36+A29 4-iodobenzoic acid					[7]
543.8	35.24	0	64.8	50.2	35.24	27.3
C_7H_5N	4*A10+2*A12+A36*B36+A29 benzotrifluoride					[7]
260.3	10.98	0	42.18	47.3	10.98	12.3
C_7H_5NO	5*A10+A12+A56 benzoxazole					[134]
247	0.02	0.07				
302.5	16.78	55.48	55.56	44.6	16.8	13.5
$C_7H_5NO_4$	A14+2*A15+2*A19+A18*B18+A112+A118+4*A10 <i>o</i> -nitrobenzoic acid					[216]
419	27.99	0	66.8	48.5	27.99	20.3
$C_7H_5NO_4$	4*A10+2*A12+A36*B36+A50 <i>m</i> -nitrobenzoic acid					[216]
414.3	19.33	0	46.66	48.5	19.33	20.1
$C_7H_5NO_4$	4*A10+2*A12+A36*B36+A50 <i>p</i> -nitrobenzoic acid					[216]
512.4	36.9	0	72.02	48.5	36.9	24.9
C_7H_5NS	4*A10+2*A12+A36*B36+A50 benzothiazole					[215]
275.6	12.8	0	46.36	46.2	12.8	12.7
$C_7H_5N_3O_6$	4*A10+A14+2*A15+A118*+2*A19+A131+A18*B18 2,4,5-trinitrotoluene					[216]
376.2	24.7	0	66.0	53.5	24.7	20.1
$C_7H_5N_3O_6$	2*A10+3*A12+3*A50*C50+A1+A11 2,4,6-trinitrotoluene					[216]
352.2	23.43	0	66.52	53.5	23.43	18.9
$C_7H_5N_5O_8$	2*A10+3*A12+3*A50*C50+A1+A11 N-methyl-2,4,6,N-tetranitroaniline					[217]
402.6	25.86	0	64.23	100.8	25.86	40.6
	4*A12+3*A50+A51+A1+2*A10+A47					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C ₇ H ₆ N ₂	benzimidazole					
	19.25	0	43.43	45.5	19.25	20.2
C ₇ H ₆ N ₂ O ₄	4*A10+A118+A121+A14+2*A15+2*A19+A18*B18					[282]
	2,4-dinitrotoluene					
C ₇ H ₆ N ₂ O ₄	20.12	0	58.61	50.7	20.12	17.4
	3*A10+A11+2*A12+2*A50+A1					[215]
C ₇ H ₆ N ₂ O ₄	2,6-dinitrotoluene					
	23.85	0	72.82	50.7	23.85	16.6
C ₇ H ₆ N ₂ O ₄	3*A10+A11+2*A12+2*A50+A1					[217]
	2,3-dinitrotoluene					
C ₇ H ₆ N ₂ O ₄	17.57	0	53.27	50.7	17.57	16.7
	3*A10+A11+2*A12+2*A50+A1					[217]
C ₇ H ₆ N ₂ O ₄	3,4-dinitrotoluene					
	18.83	0	57.15	50.7	18.83	16.7
C ₇ H ₆ N ₂ O ₅	3*A10+A11+2*A12+2*A50+A1					[217]
	2-methyl-4,6-dinitrophenol					
C ₇ H ₆ N ₂ O ₅	19.41	0	54.02	56.1	19.41	20.2
	3*A12+A11+2*A10+A1+A31+2*A50					[215]
C ₇ H ₆ O	benzaldehyde					
	9.32	0	43.1	51.1	9.32	11.0
C ₇ H ₆ O ₂	5*A10+A12+A34					[216]
	benzoic acid					
C ₇ H ₆ O ₂	18.0	0	45.45	43.0	18.0	17.0
	5*A10+A12+A36					[282]
C ₇ H ₆ O ₃	2-hydroxybenzoic acid					
	24.6	0	56.97	51.1	24.6	22.1
C ₇ H ₆ O ₃	4*A10+2*A12+A31+A36*B36					[216,8]
	3-hydroxybenzoic acid					
C ₇ H ₆ O ₃	26.2	0	55.15	51.1	26.2	24.3
	4*A10+2*A12+A31+A36*B36					[216,8]
C ₇ H ₆ O ₃	4-hydroxybenzoic acid					
	30.9	0	63.31	51.1	30.9	24.9
C ₇ H ₇ Br	4*A10+2*A12+A31+A36*B36					[233]
	benzylbromide					
C ₇ H ₇ Br	13.2	0	48.57	52.2	13.2	14.2
	5*A10+A11+A2+A21					[49]
C ₇ H ₇ Br	4-bromotoluene					
	15.13	0	50.2	47.1	15.1	14.3
C ₇ H ₇ Cl	4*A10+A11+A12+A1+A21					[234]
	<i>p</i> -chlorotoluene					
C ₇ H ₇ Cl	13.55	0	48.29	40.9	13.55	11.5
	A1+A12+A11+4*A10+A22					[234]
C ₇ H ₇ ClN ₂ S	1-(<i>o</i> -chlorophenyl)thiourea					
	22.29	0	53.91	53.9	22.29	22.3
C ₇ H ₇ F	4*A10+2*A12+A22*B22+A91					[221]
	2-fluorotoluene					
C ₇ H ₇ F	9.8	0	46.51	46.8	9.8	9.9
	4*A10+A11+A12+A1+A24					[216]
C ₇ H ₇ F	3-fluorotoluene					
	8.3	0	45.11	46.8	8.3	8.6
C ₇ H ₇ F	4*A10+A11+A12+A1+A24					[216]
	4-fluorotoluene					
C ₇ H ₇ F	9.35	0	43.18	46.8	9.35	10.13
	4*A10+A11+A1+A12+A24					[216]
C ₇ H ₇ I	benzyl iodide					
	13.2	0	44.07	54.0	13.2	16.2
C ₇ H ₇ I	5*A10+A11+A2+A29					[46]
	<i>p</i> -iodotoluene					
C ₇ H ₇ I	14.96	0	48.79	49.5	14.96	15.2
	4*A10+A11+A12+A29+A1					[234]
C ₇ H ₇ NO	benzamide					
	18.49	0	45.96	57.5	18.49	23.1
C ₇ H ₇ NO ₂	5*A10+A12+A61					[215]
	3-nitrotoluene					
C ₇ H ₇ NO ₂	19.2	0	51.88	47.9	19.2	17.7
	4*A10+A1+A11+A12+A50					[235]
C ₇ H ₇ NO ₂	4-nitrotoluene					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
318	16.9	53.1				
324.8	16.81	0	51.76	47.9	16.81	15.6
$C_7H_7NO_2$	4*A10+A12+A11+A1+A50 2-aminobenzoic acid					[215]
417.8	20.5	0	49.07	52.2	20.5	21.8
$C_7H_7NO_2$	4*A10+2*A12+A36*B36+A45 3-aminobenzoic acid					[215]
452.9	21.84	0	48.12	52.2	21.84	23.6
$C_7H_7NO_2$	4*A10+2*A12+A36*B36+A45 4-aminobenzoic acid					[215]
461.4	20.92	0	45.19	52.2	20.92	24.1
$C_7H_7NO_3$	4*A10+2*A12+A36*B36+A45 4-nitro-5-methylphenol					[215]
401	27.4	0	68.33	53.3	27.4	21.4
$C_7H_7NO_3$	3*A10+A1+A11+2*A12+A31+A50 2-nitro-5-methylphenol					[215]
302.8	20.79	0	68.66	53.3	20.79	16.1
$C_7H_7N_3O_2$	3*A10+A1+A11+2*A12+A31+A50 N-acetyl-pyrazinamide					[215]
366.7	23.6	0	64.36	61.9	23.6	22.7
C_7H_8	3*A10+A12+2*A41+A71+A1 toluene					[9]
178.0	6.62	0	37.15	45.0	6.62	8.0
C_7H_8	5*A10+A1+A11 cycloheptatriene					[216]
154.0	2.35	15.24				
198.0	1.16	5.86	21.11	38.5	3.51	7.6
C_7H_8	A14+4*A15+6*A18 tetracyclo[3.2.0.0(2,7).0(4,6)]heptane					[216]
180	7.2	40				
228	1.09	4.8	44.8	26.6	8.29	6.1
$C_7H_8N_2O$	4*A14-5*A15+6*A16 phenylurea					[216]
420.6	23.68	0	56.3	52.1	23.68	21.9
$C_7H_8N_4O_2$	5*A10+A12+A67 theophylline					[215]
544	28.2	0	51.84	44.6	28.2	24.3
546.1	28.27	0	51.76	44.6	28.3	24.3
C_7H_8O	2*A14+3*A15+2*A125+A118+A121+2*A1+2*A19+A18*B18 benzyl alcohol					[236,205]
257.6	8.79	0	34.11	36.4	8.79	9.4
C_7H_8O	5*A10+A11+A2+A30 <i>o</i> -hydroxytoluene					[215]
304.2	15.82	0	52.01	50.4	15.82	15.3
C_7H_8O	A31+A1+A12+4*A10+A11 <i>m</i> -hydroxytoluene					[216]
285.4	10.71	0	37.53	50.42	10.71	14.39
C_7H_8O	A31+A1+A12+4*A10+A11 <i>p</i> -hydroxytoluene					[216]
307.9	12.72	0	41.25	50.42	12.72	15.52
C_7H_8O	A31+A1+A12+4*A10+A11 methoxybenzene					[216]
268.7	12.9	0	48.0	51.9	12.9	13.9
C_7H_8S	5*A10+A12+A1+A32 methylphenylsulfide					[216]
256.4	14.85	0	57.86	49.3	14.85	12.63
$C_7H_9Cl_3NO_3PS$	5*A10+A12+A1+A84 O,O-dimethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate					[105]
318.7	25.92	0	81.32	73.2	25.92	23.3
$C_9H_{13}Cl_3NO_4P$	4*A12+A10+A41+3*A22*E22+2*A1+A79 O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphate					[221]
312.5	15.61	0	49.97	76.4	15.61	23.9
C_7H_9N	4*A12+A10+A41+3*A22*E22+2*A1+A74+2*A2 <i>m</i> -toluidine					[221]
241.7	8.8	0	36.41	51.5	8.8	12.5
C_7H_9N	A45+4*A10+A12+A1+A11 <i>p</i> -toluidine					[215]
316.5	17.89	0	56.52	51.5	17.89	16.3
	A45+4*A10+A12+A1+A11					[215]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C_7H_9N	<i>o</i> -toluidine					
249.6	8.08	0	32.37	51.5	8.08	12.9
	A45+4*A10+A12+A1+A11					[215]
C_7H_9N	2-methylaniline					
258	11.66	0	45.1	51.5	11.66	14.8
	4*A10+A11+A12+A1+A45					[30]
C_7H_9N	2,3-dimethylpyridine					
258.6	13.48	0	52.13	49.1	13.48	12.7
	2*A1+2*A11+3*A10+A41					[69]
C_7H_9N	2,4-dimethylpyridine					
209.4	8.82	0	42.12	49.1	8.82	10.3
	2*A1+2*A11+3*A10+A41					[69]
C_7H_9N	2,5-dimethylpyridine					
259.1	14.64	0	56.5	49.1	14.64	12.7
	2*A1+2*A11+3*A10+A41					[69]
C_7H_9N	2,6-dimethylpyridine					
267.1	13.04	0	48.82	49.1	13.04	13.1
	2*A1+2*A11+3*A10+A41					[69]
C_7H_9N	3,4-dimethylpyridine					
262.7	14.7	0	55.96	49.1	14.7	12.9
	2*A1+2*A11+3*A10+A41					[69]
C_7H_9N	3,5-dimethylpyridine					
266.9	13.11	0	49.12	49.1	13.11	13.1
	2*A1+2*A11+3*A10+A41					[69]
$C_7H_9N_5O_{12}$	2,2,2-trinitroethyl 4,4-dinitropentanoate					
363.8	20.08	55.2				
366.7	6.69	18.26	73.46	89.6	26.78	32.9
	2*A4*B4+3*A2+A1+5*A50+A38					[122]
$C_7H_9N_5O_{12}$	2,2-dinitropropyl-4,4,4-trinitrobutyrate					
284.2	25.94	91.28				
335.5	20.92	62.35				
368.2	6.69	18.18	171.8	89.6	53.56	33.0
	2*A4*B4+3*A2+A1+5*A50+A38					[122]
C_7H_{10}	bicyclo[2.2.1]hept-2-ene					
130.3	4.27	32.77				
319.5	3.48	10.89	43.66	37.8	7.75	12.1
	2*A14+A15+2*A16+2*A18					[129,349]
$C_7H_{10}O$	2-norbomanone					
368.7	3.39	0	9.19	39.7	3.39	14.6
	2*A14+A15+2*A16+A114					[217]
$C_7H_{10}N_2O$	6,7-diazatricyclo[3.2.2.0 2,4]non-6-ene-N-oxide					
372.6	15.8	42.4				
411.4	2.6	6.32	48.72	44.1	18.4	18.1
	3*A14+2*A16+2*A16+A123					[42]
$C_7H_{10}N_2O_2$	N-acetyl-L-alanine amide					
431	21.7	0	50.35	54.9	21.7	23.7
	2*A1+A60+A3*B3+A61					[278]
$C_7H_{10}N_2O_2$	1,3,6-trimethyluracil					
384.5	21.2	0	55.14	38.4	21.2	14.8
	A14+3*A15+2*A125+3*A1+A18*B18+A19					[216]
$C_7H_{10}O_3$	3,3-dimethylpentanedioic anhydride					
396.2	17.99	0	45.41	47.4	17.99	18.8
	A14+3*A15+2*A1+A17+A117					[237]
$C_7H_{11}N$	cyanocyclohexane					
215	7.43	34.53				
285.1	3.64	12.75	47.28	47.5	11.06	13.5
	A14+3*A15+A16+A56					[216]
$C_7H_{11}N$	isocyanocyclohexane					
192.6	6.18	32.07				
279.6	4.23	15.12	47.19	47.2	10.4	13.2
	A14+3*A15+A16+A57					[216]
C_7H_{12}	4-methylcyclohex-1-ene					
153.6	6.63	0	43.16	44.1	6.63	6.77
	A14+3*A15+A1+A16+2*A18					[161]
C_7H_{12}	cycloheptene					
154	5.28	34.29				
210	0.71	3.38				
217	0.97	4.47	42.14	45.0	6.96	9.8
	A14+4*A15+2*A18					[216,161]
$C_7H_{12}ClN_5$	6-chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine					
502.5	47.35	0	94.23	65.3	47.35	32.8

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (calcd)
$C_7H_{12}O_2$	3*A41+A22*F22+3*A12+2*A44+2*A1+2*A2 butyl acrylate 17.31	0	82.61	67.9	17.31	[221]
209.5						
$C_7H_{12}O_4$	A1+3*A2+A38+A5+A6*B6 pimilic acid 27.62	0	73.17	78.9	27.62	[216]
377.5						
$C_7H_{12}O_4S_2$	5*A2*B2+2*A36*B36 (dl) methylenebisthiopropionic acid 39.33	0	91.68	86.9	39.33	[340]
429						
$C_7H_{12}O_4S_2$	2*A36*D36+2*A84+2*A3*B3+2*A1+A2 (d) methylenebisthiopropionic acid 22.59	0	63.64	86.9	22.59	[273]
355						
$C_7H_{13}N$	2*A36*D36+2*A84+2*A3*B3+2*A1+A2 1-azabicyclo[2.2.2]octane 5.23	26.53				
196						
430		13.81	40.33	40.1	11.09	17.3
$C_7H_{13}NO$	2*A14+2*A15+A16+A119 ζ -enantholactam 13.78	0	44.39	54.6	13.78	[216]
310.3						
$C_7H_{13}N_3O_3S$	A14+5*A15+A124 N,N-dimethyl-2-methylcarbamoyloximino-2-(methylthio)acetamide 30.17	0	81.04	59.4	30.17	[216]
372.2						
C_7H_{14}	4*A1+A59+A7+A42+A69+A84 cycloheptane 4.98	36.94				
134.8						
198.2		1.46				
212.4		2.11				
265.1		7.1	47.6	48.2	7.6	12.8
C_7H_{14}	4*A15+A14 1,1-dimethylcyclopentane 6.49	44.18				
146.8						
203.7		5.34	49.52	41.4	7.57	8.4
C_7H_{14}	A14+A17+2*A1+2*A15 <i>cis</i> -1,2-dimethylcyclopentane 6.65	47.01				
141.5						
219.4		7.55	54.57	46.5	8.31	10.2
C_7H_{14}	A14+2*A16+2*A1+2*A15 <i>trans</i> -1,3-dimethylcyclopentane 7.4	0	53.09	46.5	7.4	[216]
139.5						
C_7H_{14}	A14+2*A16+2*A1+2*A15 ethylcyclopentane 6.87	0	51.0	50.8	6.87	[216]
134.7						
C_7H_{14}	A14+A16+A1+A2+2*A15 methylcyclohexane 6.75	0	46.1	47.3	6.75	[216]
146.6						
C_7H_{14}	A14+A16+A1+3*A15 1-heptene 12.66	0	82.5	77.5	12.66	[216]
154.3						
$C_7H_{14}NO_3P$	A1+4*A2*B2+A5+A6 dimethyl(E)-1-methyl-2-methylcarbamoylviny phosphate 22.36	0	68.4	55.0	22.36	[221]
326.9						
$C_7H_{14}N_2O_2S$	4*A1+A7+A6*B6+A60+A74 2-methyl-2(methylthio)propionaldehyde O-methylcarbamoyloxime 22.71	0	60.73	62.3	22.71	[221]
374.0						
$C_7H_{13}N_3O_3S$	4*A1+A4*B4+A6*B6+A69+A84+A42 N,N-dimethyl-2-methylcarbamoyloximino-2-(methylthio)acetamide 30.17	0	81.05	59.4	30.17	[221]
372.2						
$C_7H_{14}O$	4*A1+A59+A7+A84+A42+A69 heptanal 22.89	0	99.83	85.8	22.89	[43]
229.3						
$C_7H_{14}O$	A1+5*A2*B2+A34 diisopropyl ketone 11.2	0	54.6	55.3	11.2	[216]
204.8						
$C_7H_{14}O$	4*A1+2*A3*B3+A35 1-methylcyclohexanol 10.87	0	36.34	29.2	10.87	[230]
299.2						
$C_7H_{14}O$	A14+3*A15+A1+A17+A30 cycloheptanol 2.93	16.98				
172.2						

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
227.3	0.55	2.44				
258.4	0.88	3.39				
280.3	1.6	5.72	28.53	35.2	5.96	9.9
$C_7H_{14}O_2$	A 14 + 4*A 15 + A 30 + A 16					
	heptanoic acid					
	224.8	2.04	9.08			
265.8	15.44	58.07	67.15	77.6	17.48	20.6
$C_7H_{15}Cl_2N_2O_2P$	5*A 2*B 2 + A 1 + A 36					
	2-[bis(2-chloroethyl)amino]tetrahydro-2H-1,3,2-oxazophosphorine-2-oxide					
322.6	33.13	0	102.7	102.7	33.13	33.1
C_7H_{16}	A 14 + 3*A 15 + A 144 + 4*A 2 + 2*A 22*C 22					
	heptane					
182.6	14.04	0	76.9	81.8	14.04	14.9
C_7H_{16}	2*A 1 + 5*A 2*B 2					
	2,4-dimethylpentane					
154.0	6.85	0	44.46	44.7	6.85	6.9
C_7H_{16}	4*A 1 + A 2 + 2*A 3					
	3-ethylpentane					
154.6	9.55	0	61.77	57.8	9.55	8.9
C_7H_{16}	3*A 1 + 3*A 2 + A 3					
	2-methylhexane					
154.9	9.18	0	59.29	57.8	9.18	9.0
C_7H_{16}	3*A 1 + 3*A 2 + A 3					
	3,3-dimethylpentane					
138.2	7.07	0	51.16	49.7	7.07	6.9
C_7H_{16}	4*A 1 + A 4 + 2*A 2					
	2,2,3-trimethylbutane					
121	2.38	19.64				
247.7	2.2	8.88	28.53	36.7	4.58	4.4
C_7H_{16}	5*A 1 + A 3 + A 4					
	2,2-dimethylpentane					
148.1	5.86	0	39.55	49.74	5.86	7.37
$C_7H_{16}O$	4*A 1 + A 4 + 2*A 2					
	1-heptanol					
240.4	18.16	0	75.53	75.31	18.16	18.1
$C_7H_{16}O_2$	A 1 + 6*A 2*B 2 + A 30					
	1,7-heptanediol					
295.2	21.3	0	72.15	101.6	21.3	30.0
$C_7H_{16}S$	7*A 2*B 2 + 2*A 30*B 30					
	1-heptanethiol					
229.9	25.4	0	110.4	96.6	25.4	22.2
$C_7H_{17}NSi$	A 1 + 6*A 2*B 2 + A 86					
	N-(β -trimethylsilyethyl)ethylenimine					
176.5	10.62	0	60.17	54.0	10.62	9.5
$C_7H_{20}Si_2$	3*A 1 + 2*A 2 + A 14 + A 119 + A 109					
	hexamethyldisilylmethane					
140.7	11.11	0	78.98	58.5	11.11	8.2
$C_8Cl_4N_2$	6*A 1 + 2*A 109 + A 2					
	2,4,5,6-tetrachloro-1,3-benzenedicarbonitile					
526.2	30	0	57.01	55.3	30	29.1
C_8F_{18}	4*A 22*F 22 + 2*A 56 + 6*A 12					
	perfluorooctane					
176.5	3.14	17.79				
254.2	9.58	37.69	55.48	93.8	12.72	23.8
$C_8H_3NO_5$	8*A 4*B 4 + 12*A 26 + 6*A 25					
	3-nitrophthalic anhydride					
436.2	18.4	0	42.18	51.0	18.4	22.3
$C_8H_3NO_5$	A 14 + 2*A 15 + A 117 + 2*A 19 + A 12 + 3*A 10 + A 50					
	4-nitrophthalic anhydride					
388.2	17.14	0	44.15	51.0	17.14	19.8
$C_8H_4Cl_2O_2$	A 14 + 2*A 15 + A 117 + 2*A 19 + A 12 + 3*A 10 + A 50					
	terephthalyl dichloride					
337.3	2.34	6.92				
356.1	21.1	59.25	66.18	66.2	23.44	23.6
$C_8H_4N_2$	4*A 10 + 2*A 12 + 2*A 40					
	1,2-dicyanobenzene					
414.1	20	0	48.3	50.2	20	20.8
$C_8H_4O_3$	4*A 10 + 2*A 12 + 2*A 56					
	phthalic anhydride					
403.3	23.09	0	57.25	48.2	23.09	19.4
	A 14 + 2*A 15 + 2*A 19 + A 117 + 4*A 10					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_8\text{H}_5\text{Cl}_3\text{O}_2$	2,3,6-trichlorophenylacetic acid 22.43	0	51.89	68.5	22.43	29.6
	$2^*A10+3^*A12+A11+A36^*D36+3^*A22^*D22+A2$					[215]
$\text{C}_8\text{H}_5\text{Cl}_3\text{O}_3$	(2,4,5-trichlorophenoxy)acetic acid 38	0	88.13	75.3	38	32.5
	$3^*A22^*E22+A32+A36^*E36+4^*A12+2^*A10+A2$					[215]
$\text{C}_8\text{H}_5\text{Cl}_3\text{O}_4$	3,6-dichloro-5-hydroxy-2-methoxybenzoic acid 28.98	0	70.7	75.0	28.98	30.7
	$2^*A22^*E22+A31+A32+A36^*E36+5^*A12+A10+A1$					[215]
C_8H_6	phenylacetylene 9.46	0	41.49	41.7	9.46	9.5
	$5^*A10+A12+A8+A9$					[132]
$\text{C}_8\text{H}_6\text{Cl}_2\text{O}_3$	(2,4-dichlorophenoxy)acetic acid 35.33	0	85.64	74.0	35.33	30.5
	$3^*A10+3^*A12+A2+2^*A22^*D22+A36^*D36+A32^*D32$					[221]
$\text{C}_8\text{H}_6\text{Cl}_2\text{O}_3$	3,6-dichloro-2-methoxybenzoic acid 22.9	0	59.23	69.6	22.9	26.9
	$4^*A12+2^*A10+2^*A22^*D22+A36^*D36+A32^*D32+A1$					[215]
$\text{C}_8\text{H}_6\text{Cl}_2\text{O}_3$	2,4-dichloro-2-methoxybenzoic acid 35.33	0	85.65	69.6	35.33	28.7
	$4^*A12+2^*A10+2^*A22^*D22+A36^*D36+A32^*D32+A1$					[215]
$\text{C}_8\text{H}_6\text{Cl}_2\text{O}_4$	3,6-dichloro-5-hydroxy-2-methoxybenzoic acid 28.98	0	70.71	75.0	28.98	30.7
	$A10+5^*A12+2^*A22^*E22+A36^*E36+A1+A32+A31$					[215]
$\text{C}_8\text{H}_6\text{Cl}_4$	tetrachloro- <i>o</i> -xylene 21.46	0	59.74	50.8	21.46	18.2
	$4^*A12+2^*A11+2^*A1+4^*A22^*D22$					[215]
$\text{C}_8\text{H}_6\text{Cl}_4$	tetrachloro- <i>p</i> -xylene 22.59	0	61.35	50.8	22.59	18.7
	$4^*A12+2^*A11+2^*A1+4^*A22^*D22$					[215]
$\text{C}_8\text{H}_6\text{Cl}_4\text{O}_4$	methyl tetrachloroterephthalic acid ester 16.89	0	38.03	92.7	16.89	41.2
	$6^*A12+2^*A1+A38+4^*A22^*F22+A36$					[221]
$\text{C}_8\text{H}_6\text{N}_2$	phthalazine 13.32	0	36.54	51.4	13.32	18.7
	$6^*A10+2^*A12+2^*A41$					[29]
$\text{C}_8\text{H}_6\text{N}_2$	quinazoline 16.95	0	52.82	51.4	16.95	16.5
	$6^*A10+2^*A12+2^*A41$					[29]
$\text{C}_8\text{H}_6\text{N}_2$	quinoxaline 11.80	0	38.61	51.4	11.80	15.7
	$6^*A10+2^*A12+2^*A41$					[29]
$\text{C}_8\text{H}_6\text{N}_2\text{OS}_2$	6-methyl-1,3-dithiolo[4,5- <i>b</i>]quinoxalin-2-one 29.92	0	67.49	67.5	29.92	29.9
	$A14+2^*A15+A135+2^*A19+2^*A41+A1+A11$ $+3^*A10+2^*A12$					[221]
$\text{C}_8\text{H}_6\text{S}$	benzothiophene 11.82	0	38.82	44.1	11.82	13.4
	$4^*A10+A14+2^*A15+A19+A18+A131+A19+A18^*B18$					[95]
$\text{C}_8\text{H}_7\text{ClO}_3$	(<i>d</i>) <i>o</i> -chloromandelic acid 24.69	0	62.89	66.1	24.69	25.9
	$4^*A10+A11+A12+A3^*B3+A30^*C30+A36^*C36+A22^*C22$					[220]
$\text{C}_8\text{H}_7\text{ClO}_3$	(<i>dl</i>) <i>o</i> -chloromandelic acid 20.08	0	56.02	66.0	20.08	23.6
	$4^*A10+A11+A12+A3^*B3+A30^*C30+A36^*C36+A22^*C22$					[220]
$\text{C}_8\text{H}_7\text{ClO}_3$	(<i>dl</i>) <i>p</i> -chloromandelic acid 27.2	0	69.03	66.0	27.2	26.0
	$4^*A10+A12+A11+A3^*B3+A30^*C30+A36^*C36+A22^*C22$					[220]
$\text{C}_8\text{H}_7\text{ClO}_3$	(<i>d</i>) <i>p</i> -chloromandelic acid 23.01	0	58.41	66.0	23.01	26.0
	$4^*A10+A11+A12+A3^*B3+A30^*C30+A36^*C36+A22^*C22$					[220]
$\text{C}_8\text{H}_7\text{Cl}_2\text{NO}$	methyl-3,4-dichlorophenylcarbamate 23.19	0	60.8	60.4	23.19	23.0
	$A1+3^*A10+3^*A12+2^*A22^*C22+A69$					[221]
$\text{C}_8\text{H}_7\text{FO}_3$	(<i>dl</i>) <i>m</i> -fluoromandelic acid 24.69	0	66.72	66.4	24.69	24.6

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)	
$\text{C}_8\text{H}_7\text{FO}_3$	4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24 (<i>d</i>) <i>m</i> -fluoromandelic acid	24.27	0	61.59	66.4	24.27	[220,187]
$\text{C}_8\text{H}_7\text{FO}_3$	4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24 (<i>dl</i>) <i>o</i> -fluoromandelic acid	30.12	0	77.24	66.4	30.12	[220,187]
$\text{C}_8\text{H}_7\text{FO}_3$	4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24 (<i>d</i>) <i>o</i> -fluoromandelic acid	20.92	0	57.63	66.4	20.92	[220,187]
$\text{C}_8\text{H}_7\text{FO}_3$	4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24 (<i>dl</i>) <i>p</i> -fluoromandelic acid	29.29	0	72.67	66.4	29.29	[220,187]
$\text{C}_8\text{H}_7\text{FO}_3$	4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24 (<i>d</i>) <i>p</i> -fluoromandelic acid	30.54	0	71.7	66.4	30.54	[220,187]
$\text{C}_8\text{H}_7\text{ClO}_3$	4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24 4-chlorophenoxyacetic acid	36.27	0	84.42	72.8	36.27	[220,187]
$\text{C}_8\text{H}_7\text{N}_3\text{O}_6$	4*A10+2*A12+A22*C22+A36*C36+A2+A32 2,4,6-trinitro-1,3-dimethylbenzene	38.49	0	84.52	54.1	38.49	[221]
$\text{C}_8\text{H}_7\text{N}_5\text{O}_8$	A10+2*A11+3*A12+2*A1+3*A50 2,4,6-N-tetranitro-N-methyltoluidene	19.33	0	51.46	54.3	19.33	[197]
$\text{C}_8\text{H}_7\text{N}_5\text{O}_8$	4*A12+A10+A11+3*A50+2*A1+A51+A49 2,4,6-N-tetranitroethylaniline	23.51	0	63.6	60.8	23.51	[216]
C_8H_8	A51+4*A12+2*A10+A1+A2+3*A50+A49 cubane	5.94	15.08				
C_8H_8	5*A14-7*A15+8*A16 styrene	8.7	21.49	36.56	23.2	14.64	[150]
C_8H_8	5*A10+A5+A6+A12 cyclooctatetraene	11.27	0	41.49	39.0	11.27	[216]
$\text{C}_8\text{H}_8\text{BrCl}_2\text{O}_3\text{PS}$	A14+5*A15+8*A18 O-(4-bromo-2,5-dichlorophenyl)O,O-dimethyl phosphorothioate	31.15	0	95.74	71.1	31.15	[216]
$\text{C}_8\text{H}_8\text{Br}_2$	2*A10+4*A12+2*A1+2*A22*D22+A21+A79 α, α' -dibromo- <i>o</i> -xylene	26.78	0	72.73	59.8	26.78	[221]
$\text{C}_8\text{H}_8\text{Br}_2$	4*A10+2*A11+2*A2+2*A21*B21 α, α' -dibromo- <i>m</i> -xylene	23.69	0	67.65	59.8	23.69	[215]
$\text{C}_8\text{H}_8\text{ClNO}_2$	4*A10+2*A11+2*A2+2*A21*B21 N-methyl-2-chlorophenylcarbamic acid ester	21.81	0	60.12	59.1	21.81	[215]
$\text{C}_8\text{H}_8\text{Cl}_2$	A1+4*A10+2*A12+A69+A22*B22 α, α' -dichloro- <i>o</i> -xylene	21.26	0	64.78	57.1	21.26	[221]
$\text{C}_8\text{H}_8\text{Cl}_2$	4*A10+2*A11+2*A2+2*A22*B22 α, α' -dichloro- <i>m</i> -xylene	19.51	0	63.51	57.1	19.51	[215]
$\text{C}_8\text{H}_8\text{Cl}_2$	4*A10+2*A11+2*A2+2*A22*B22 α, α' -dichloro- <i>p</i> -xylene	23.97	0	64.23	57.1	23.97	[215]
$\text{C}_8\text{H}_8\text{Cl}_2\text{O}_2$	4*A10+2*A11+2*A2+2*A22*B22 1,4-dichloro-2,5-dimethoxybenzene	27.56	0	68.23	61.8	27.56	[215]
$\text{C}_8\text{H}_8\text{Cl}_2\text{O}_3$	4*A12+2*A10+2*A22*D22+2*A32*D32+2*A1 methyl 3,6-dichloro-2-methoxybenzoate	18.49	0	60.72	64.8	18.49	[215]
$\text{C}_8\text{H}_8\text{Cl}_3\text{O}_3\text{PS}$	2*A10+4*A12+2*A1+2*A22*D22+A38*D38+A32*D32 O,O-dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate						[221]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
313.0	18.94	0	60.51	69.7	18.94	21.8
$\text{C}_8\text{H}_8\text{O}_2$	2*A10+4*A12+3*A22*D22+2*A1+A79 <i>o</i> -toluic acid					[221]
376.9	20.17	0	53.51	43.5	20.17	16.4
$\text{C}_8\text{H}_8\text{O}_2$	4*A10+A12+A11+A1+A36 <i>m</i> -toluic acid					[215]
381.9	15.73	0	41.19	43.5	15.73	16.6
$\text{C}_8\text{H}_8\text{O}_2$	4*A10+A12+A11+A1+A36 <i>p</i> -toluic acid					[215]
452.8	22.72	0	50.17	43.5	22.72	19.7
$\text{C}_8\text{H}_8\text{O}_2$	4*A10+A12+A11+A1+A36 phenylacetic acid					[215]
349.9	14.49	0	41.41	48.0	14.49	16.8
$\text{C}_8\text{H}_8\text{O}_2$	5*A10+A11+A2+A36 methyl benzoate					[215]
261	13.9	0	53.26	54.8	13.9	14.3
$\text{C}_8\text{H}_8\text{O}_2\text{S}$	5*A10+A1+A38+A12 phenyl vinyl sulfone					[247]
343.4	11.72	0	34.12	52.5	11.72	18.0
$\text{C}_8\text{H}_8\text{O}_3$	5*A10+A5+A6+A12+A88 methyl 4-hydroxybenzoate					[238]
398.5	24.31	0	61	60.2	24.31	24.0
$\text{C}_8\text{H}_8\text{O}_3$	4*A10+2*A12+A1+A31+A38*B38 (<i>dl</i>) mandelic acid					[239]
392	25.52	0	65.11	51.9	25.52	20.3
$\text{C}_8\text{H}_8\text{O}_3$	5*A10+A3*B3+B30*A30+A36*B36+A11 (<i>d</i>) mandelic acid					[220]
406	23.36	0	64.92	51.9	26.36	21.1
$\text{C}_8\text{H}_8\text{O}_3$	5*A10+A3*B3+B30*A30+A36*B36+A11 4-hydroxyphenylacetic acid					[220]
423.6	28.4	0	67.04	56.1	28.4	23.9
$\text{C}_8\text{H}_8\text{O}_3$	4*A10+A11+A12+A2+A36*B36+A31 4-methoxybenzoic acid					[215]
457.8	28.4	0	62.04	53.1	28.4	24.3
455.4	27.8	0	61.1	53.1	27.8	23.9
$\text{C}_8\text{H}_9\text{ClO}_3$	4*A10+2*A12+A1+A36*B36+A32 (4-chloro-2-methylphenoxy)acetic acid					[215,394]
392.9	29.98	0	76.31	73.3	29.98	28.8
$\text{C}_8\text{H}_9\text{NO}$	3*A10+2*A12+A11+A22*C22+A36*C36+A32+A2+A1 4-aminoacetophenone					[221]
379.2	38	0	100.2	58.2	38	22.1
$\text{C}_8\text{H}_9\text{NO}$	4*A10+2*A12+A35+A45+A1 3-aminoacetophenone					[280]
371.2	29	0	78.12	58.2	29	21.6
$\text{C}_8\text{H}_9\text{NO}$	4*A10+2*A12+A35+A45+A1 acetanilide					[280]
387.5	21.65	0	55.87	48.6	21.6	18.8
$\text{C}_8\text{H}_9\text{NO}_2$	5*A10+A12+A1+A60 methyl 4-aminobenzoate					[216]
385.1	22.55	0	58.56	61.3	22.55	23.6
$\text{C}_8\text{H}_9\text{NO}_2$	4*A10+2*A12+A1+A45+A38 <i>o</i> -hydroxyacetanilide					[239]
364.5	21.25	0	58.3	54.0	21.25	23.8
$\text{C}_8\text{H}_9\text{NO}_2$	4*A10+A60+A1+2*A12+A31 <i>p</i> -hydroxyacetanilide					[216]
441.2	26.02	0	58.99	54.0	26.02	23.8
441.7	27.0	0	60.9	54.0	27.0	23.8
$\text{C}_8\text{H}_9\text{NO}_2$	4*A10+A60+A1+2*A12+A31 methyl <i>N</i> -phenylcarbamate					[239,394]
325	14.56	0	44.77	57.8	14.56	18.8
$\text{C}_8\text{H}_9\text{ClNO}_5\text{PS}$	5*A10+A12+A1+A69 O-(2-chloro-4-nitrophenyl)O,O-dimethyl phosphorothioate					[216]
323.9	29.08	0	89.78	70.0	29.08	22.7
$\text{C}_8\text{H}_9\text{O}_3\text{PS}$	2*A1+3*A10+3*A12+A22*C22+A50+A79 2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulfide					[221]
327.86	16.92	0	51.61	51.6	16.92	16.9

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
C_8H_{10}	A14+3*A15+A19+A19+4*A10+A130+A1					[221]
247.8	<i>o</i> -xylene 13.6	0	54.9	45.6	13.6	11.3
C_8H_{10}	2*A1+4*A10+2*A11					[216]
225.3	<i>m</i> -xylene 11.57	0	51.4	45.6	11.57	10.3
C_8H_{10}	2*A1+4*A10+2*A11					[216]
286.3	<i>p</i> -xylene 17.11	0	59.77	45.6	17.11	13.1
C_8H_{10}	2*A1+4*A10+2*A11					[216]
178.2	ethylbenzene 9.16	0	51.43	52.2	9.16	9.3
$C_8H_{10}N_4O_2$	A1+A2+5*A10+A11					[216]
426	caffeine 0.94	2.21				
512	23.43	45.76	47.97	40.7	24.37	20.9
510.1	18.3	35.88	38.1	40.7	19.4	20.9
$C_8H_{10}NO_3PS$	2*A14+3*A15+2*A125+3*A1+2*A19+A18*B18+A119+A118					[227,395]
308.2	O,O-dimethyl O-4-nitrophenyl phosphorothioate 20.07	0	65.12	68.7	20.07	21.2
$C_8H_{10}O$	4*A10+2*A12+2*A1+A50+A79					[215]
346	2,3-dimethylphenol 21.02	0	60.75	51.0	21.02	17.6
$C_8H_{10}O$	3*A10+2*A11+A12+2*A1+A31					[215]
348	2,5-dimethylphenol 23.38	0	67.18	51.0	23.38	17.7
$C_8H_{10}O$	3*A10+2*A11+A12+2*A1+A31					[215]
318.9	2,6-dimethylphenol 18.9	0	59.27	51.0	18.9	16.3
$C_8H_{10}O$	3*A10+2*A11+A12+2*A1+A31					[215]
334	3,4-dimethylphenol 18.13	0	54.28	51.0	18.13	17.0
$C_8H_{10}O$	3*A10+2*A11+A12+2*A1+A31					[215]
336.8	3,5-dimethylphenol 18	0	53.44	51.0	18.0	17.2
$C_8H_{10}O_2S$	3*A10+2*A11+A12+2*A1+A31					[215]
400.5	benzylmethylsulfone 25.52	0	63.73	52.5	25.52	21.0
$C_8H_{11}N$	5*A10+A11+A1+A2+A88					[276]
279	2,5-dimethylaniline 13.7	0	49.1	52.1	13.7	14.5
$C_8H_{11}N$	3*A10+2*A11+A12+2*A1+A45					[51]
275.6	N,N-dimethylaniline 11.56	0	46.28	42.5	11.56	11.7
$C_8H_{11}N$	5*A10+A12+A43+2*A1					[51]
237.7	exo-2-cyanobicyclo[2.2.1]heptane 7.93	33.4				
298.8	2.94	9.83	43.2	44.0	10.87	13.1
$C_8H_{11}N$	2*A14+A15+2*A16+A16+A56					[216]
177.3	endo-2-cyanobicyclo[2.2.1]heptane 2.25	12.7				
331.2	2.96	8.94	21.6	44.0	7.18	14.6
$C_8H_{11}N$	2*A14+A15+2*A16+A56+A16					[216]
229.0	2,4,6-trimethylpyridine 9.54	0	41.64	50.0	9.54	11.4
$C_8H_{11}N_5$	3*A1+3*A11+2*A10+A41					[216]
438	6,8,9-trimethyladenine 23.1	0	52.74	54.4	23.1	23.8
$C_8H_{11}N_5O_2$	A14+2*A15+3*A19+3*A1+A118+A119+2*A41+A10+A12+A44					[240]
462.2	2-amino-9-[(2-hydroxyethoxy)methyl]-9H-purine 42.2	0	91.3	86.5	42.2	40.0
$C_8H_{11}N_5O_3$	A14+2*A15+2*A19+A18*B18+2*A41+A45+A118+A119+3*A2+A30*F30+A32					[203]
528.2	2-amino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one 30.44	0	57.63	92.7	30.44	48.9

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
C_8H_{12}	$2*A14+3*A15+3*A19+A18*B18+A124+2*A118+A45+A119+3*A2+A32+A30*F30$					[203]
	2-bicyclo[2.2.2]octene					
110.5	0.19	1.7				
176.5	5.65	32				
389.8	5.4	13.85	47.55	41.5	11.23	16.2
C_8H_{12}	$2*A14+2*A15+2*A16+2*A18$					[100]
	cycloocta-1,5-diene					
194.4	-0.38	9.83	48.2	45.4	9.83	9.3
204		0				[216]
$C_8H_{12}NO_5PS_2$	$A14+5*A15+4*A18$					[216]
	O,O-dimethyl O-(4-aminosulfonylphenyl)phosphorodithioate					
344.2	26.21	0	76.13	79.4	26.21	27.3
$C_8H_{12}N_2$	$2*A1+4*A10+2*A12+A96+A79$					[221]
	tetramethylsuccinonitrile					
345	18.1	52.48				
442	7.15	16.17	68.64	60.1	25.25	26.6
$C_8H_{12}N_2O_2$	$4*A1+2*A4*B4+2*A56$					[216]
	1,6-hexamethylene diisocyanate					
206.1	18.64	0	90.46	102.2	18.64	21.1
$C_8H_{12}N_2O_3$	$6*A2*B2+2*A58$					[216]
	barbitol					
462.6	24.98	0	54	63.1	24.98	29.2
$C_8H_{12}N_4O_{10}$	$A14+3*A15+A128+A124+2*A1+2*A2+A17$					[241]
	2,2-dinitropropyl 4,4-dinitropentanoate					
330.6	23.01	69.61				
370.8	6.28	16.93	86.53	89.4	29.29	33.2
$C_8H_{12}N_4O_{10}$	$2*A4*B4+3*A2+2*A1+4*A50+A38$					[122]
	2-methyl-2-nitropropyl 4,4,4-trinitrobutyrate					
346.1	24.69	71.33				
349.4	5.27	15.09	86.41	89.4	29.96	31.3
$C_8H_{12}O_2$	$2*A1+2*A4*B4+3*A2+4*A50+A38$					[122]
	1,4-cyclooctanedione					
341.2	11.92	0	34.95	49.2	11.92	16.8
$C_8H_{13}ClN_2O_2$	$A14+5*A15+2*A114$					[114]
	5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione					
448	12.51	0	27.92	64.6	12.51	28.9
C_8H_{14}	$A14+3*A15+2*A19+A124+A125+4*A1+A4*B4+A22*C22$					[221]
	endo-2-methylbicyclo[2.2.1]heptane					
152.4	4.71	30.9				
278.3	1.62	5.82	36.72	43.8	6.35	12.2
C_8H_{14}	$2*A14+A15+A1+3*A16$					[216]
	exo-2-methylbicyclo[2.2.1]heptane					
164.1	8.38	0	51.0	43.8	8.38	7.2
C_8H_{14}	$2*A14+A15+A1+3*A16$					[216]
	bicyclo[2.2.2]octane					
164.3	4.6	28.01				
447.5	8.37	18.7	46.71	44.7	12.97	20.0
C_8H_{14}	$2*A14+2*A16+2*A15$					[215]
	cyclooctene					
190.1	9.8	51.55				
259.2	1.81	6.98	58.53	48.7	11.61	12.6
$C_8H_{14}N_4OS$	$A14+5*A15+2*A18$					[161]
	4-amino-6-(1,1-dimethylethyl)-3-(methylthio)1,2,4-triazin-5(4H)-one					
399.4	18	0	45.06	58.2	18	23.3
$C_8H_{14}N_5Cl$	$A14+3*A15+2*A19+4*A1+A4+A125+A84+A45+2*A118$					[215]
	6-chloro-N-ethyl-N'-(isopropyl)-1,3,5-triazine-2,4-diamine					
449.7	38.15	0	84.84	65.9	38.15	29.7
$C_8H_{14}N_6O_{10}$	$3*A41+3*A12+2*A44+A22*F22+3*A1+A2+A3*B3$					[221]
	1,7-diacetoxy-2,4,6-trinitro-2,4,6-triazahseptane					
422.5	38.49	0	91.11	214.5	38.49	90.6
$C_8H_{14}O$	$2*A1+4*A2+2*A38+3*A51+3*A47$					[216]
	3-oxabicyclo[3.2.2]nonane					
208.5	7.02	33.65				
448.4	6.75	15.06	48.71	49.6	13.77	22.3
$C_8H_{14}O_4$	$2*A14+3*A15+2*A16+A112$					[216]
	suberic acid					
415.3	28.82	0	69.4	88.2	28.82	36.6
	$6*A2*B2+2*A36*B36$					[340]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_8H_{14}O_4$	tetramethylsuccinic acid					
383	13.43	35.07				
464	6.47	13.95	49.02	56.8	19.9	26.4
	$4*A1 + 2*A4*B4 + 2*A36*B36$					[216]
$C_8H_{15}N$	3-azabicyclo[3.2.2]nonane					
297.8	14.55	48.87				
466.6	6.92	14.82	63.69	50.6	21.47	23.6
	$2*A14 + 3*A15 + 2*A16 + A121$					[216]
$C_8H_{15}NO_2$	dimethylaminoethyl methacrylate					
237.7	16.85	0	70.9	59.1	16.85	14.0
	$3*A1 + 2*A2 + A5 + A7 + A38 + A43$					[216]
C_8H_{16}	cyclooctane					
166.5	6.32	37.94				
183.8	0.48	2.6				
288	2.41	8.35	48.89	51.9	9.2	14.9
	$5*A15 + A14$					[215]
C_8H_{16}	1,1-dimethylcyclohexane					
153.2	5.98	39.05				
239.8	2.01	8.37	47.43	45.1	7.99	10.8
	$A14 + A17 + 2*A1 + 3*A15$					[216]
C_8H_{16}	propylcyclopentane					
155.8	10.04	0	64.45	57.9	10.04	9.0
	$A14 + A16 + A1 + 2*A2 + 2*A15$					[216]
C_8H_{16}	<i>trans</i> -1,2-dimethylcyclohexane					
185	10.5	0	56.77	50.2	10.5	9.3
	$A14 + 3*A15 + 2*A1 + 2*A16$					[216]
C_8H_{16}	<i>cis</i> -1,2-dimethylcyclohexane					
172.5	8.26	47.86				
223.3	1.64	7.36	55.22	50.2	9.9	11.2
	$A14 + 3*A15 + 2*A1 + 2*A16$					[216]
C_8H_{16}	<i>trans</i> -1,3-dimethylcyclohexane					
183.1	9.87	0	53.93	50.2	9.87	9.2
	$A14 + 3*A15 + 2*A1 + 2*A16$					[216]
C_8H_{16}	<i>cis</i> -1,3-dimethylcyclohexane					
197.6	10.82	0	54.77	50.2	10.82	9.9
	$A14 + 3*A15 + 2*A1 + 2*A16$					[216]
C_8H_{16}	<i>trans</i> -1,4-dimethylcyclohexane					
236.2	12.34	0	52.26	50.2	12.34	11.9
	$A14 + 3*A15 + 2*A1 + 2*A16$					[216]
C_8H_{16}	<i>cis</i> -1,4-dimethylcyclohexane					
185.7	9.31	0	50.11	50.2	9.31	9.3
	$A14 + 3*A15 + 2*A1 + 2*A16$					[216]
C_8H_{16}	ethylcyclohexane					
161.4	8.28	0	51.3	54.5	8.28	8.8
	$A14 + A16 + A1 + A2 + 3*A15$					[216]
C_8H_{16}	1-octene					
171.5	15.31	0	89.29	86.8	15.31	14.9
	$A1 + 5*A2*B2 + A5 + A6$					[216]
C_8H_{16}	2,4,4-trimethyl-1-pentene					
178.9	8.77	0	49.0	49.2	8.77	8.8
	$4*A1 + A2 + A5 + A7 + A4$					[216]
C_8H_{16}	2,4,4-trimethyl-2-pentene					
166	6.8	0	40.9	47.6	6.78	7.9
	$5*A1 + A4 + A7 + A6$					[216]
$C_8H_{16}N_2O_2$	N-acetyl-D-leucine amide					
404	20.2	0	50	63.2	20.2	25.5
	$3*A1 + A3 + A3*B3 + A2 + A61 + A60$					[216]
$C_8H_{16}N_6$	1-(methylamino)-3,5-bis(dimethylamino)-s-triazine					
378.8	22.34	0	58.98	48.4	22.34	18.3
	$3*A41 + 3*A12 + 2*A43 + A44 + 5*A1$					[242]
$C_8H_{16}N_6O$	1-(hydroxylamino)-3,5-bis(dimethylamino)-s-triazine					
381.5	30.67	0	80.39	53.6	30.67	20.4
	$4*A1 + 3*A41 + 3*A12 + 2*A43 + A30*F30 + A44$					[242]
$C_8H_{16}O$	octanal					
288.2	25.86	0	89.73	95.1	25.86	27.4
	$6*A2*B2 + A1 + A34$					[93]
$C_8H_{16}O$	2-octanone					
252.86	24.42	0	96.57	86.4	24.42	21.8

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_8\text{H}_{16}\text{O}_2$	289.7	0	73.8	86.9	21.35	25.2
	2*A1 + 5*A2*B2 + A35 octanoic acid 21.35					[216]
$\text{C}_8\text{H}_{16}\text{O}_2$	250.6	0	43.5	48.1	10.9	12.1
	6*A2*B2 + A1 + A36 2,2,6,6-tetramethyl-1,3-dioxane 10.9					[216]
$\text{C}_8\text{H}_{16}\text{O}_2$	181.68	0	82.18	78.5	14.93	14.3
	A14 + 3*A15 + 2*A112 + 4*A1 + 2*A17 butyl butanoate 14.93					[47]
$\text{C}_8\text{H}_{16}\text{O}_2$	212.1	0	93.49	89.5	19.83	19.0
	2*A1 + 5*A2 + A38 hexyl ethanoate 19.83					[216]
C_8H_{18}	216.38	0	95.86	91.1	20.74	19.7
	2*A1 + 5*A2*B2 + A38 <i>n</i> -octane 20.74					[216]
C_8H_{18}	165.3	0	54.7	43.8	9.04	7.3
	2*A1 + 6*A2*B2 2,2,4-trimethylpentane 9.04					[216]
C_8H_{18}	165.8	0	55.52	43.8	9.2	7.3
	5*A1 + A4 + A2 + A3 2,2,4-trimethylpentane 9.2					[216]
C_8H_{18}	163.6	0	56.65	38.8	9.27	6.4
	5*A1 + A2 + A4 + A3 2,3,4-trimethylpentane 9.27					[216]
C_8H_{18}	152.6	0	76.6	64.9	11.7	9.9
	5*A1 + 3*A3 3-methylheptane 11.7					[216]
C_8H_{18}	164.2	0	72.62	64.9	11.92	10.7
	3*A1 + 4*A2 + A3 2-methylheptane 11.92					[216]
C_8H_{18}	152.5	13.11				
373.9	7.54	20.16	33.28	35.8	9.54	13.4
	3*A1 + 4*A2 + A3 2,2,3,3-tetramethylbutane 7.54					[216]
C_8H_{18}	152.2	0	71.22	64.9	10.84	9.9
	6*A1 + 2*A4 4-methylheptane 10.84					[215]
$\text{C}_8\text{H}_{18}\text{Cl}_2\text{Sn}$	316.2	0	71.95	86.1	22.75	27.2
	3*A1 + A3 + 4*A2 di- <i>n</i> -butyltindichloride 22.75					[130]
$\text{C}_8\text{H}_{18}\text{N}_2$	242.6	20.16				
258.6	10.28	39.75	59.91	56.3	15.17	14.6
	2*A1 + 6*A2 + 2*A2*D22 + A110 1,1-dimethylazoethane 4.89					[42]
$\text{C}_8\text{H}_{18}\text{N}_2\text{O}$	268	31.12				
288.4	11.52	39.94	71.06	64.9	19.86	18.7
	6*A1 + 2*A4*B4 + 2*A42 1,1-dimethylazoxyethane 8.34					[42]
$\text{C}_8\text{H}_{18}\text{N}_2\text{O}_2$	405	0	63.95	80.2	25.9	32.5
	6*A1 + 2*A4*B4 + A54 + A42 <i>bis</i> -hydroxyethylpiperazine 25.9					[216]
$\text{C}_8\text{H}_{18}\text{N}_4\text{O}_4$	331	0	186.35	113.0	61.68	37.4
	A14 + 3*A15 + 2*A119 + 4*A2 + 2*A30*D30 N,N'-dimethyl-N,N'-dinitro-1,6-hexanediamine 61.68					[225]
$\text{C}_8\text{H}_{18}\text{O}_2$	332.8	0	108.47	111.0	36.1	36.9
	6*A2 + 2*A1 + 2*A43 + 2*A51 1,8-octanediol 36.1					[215]
$\text{C}_8\text{H}_{18}\text{O}_4$	229.3	0	103.34	96.8	23.71	22.2
	8*A2*B2 + 2*A30*B30 2,5,8,11-tetraoxadodecane 23.71					[216]
$\text{C}_8\text{H}_{18}\text{S}$	198.1	0	93.85	80.1	19.41	15.9
	2*A1 + 6*A2 + 4*A32 di- <i>n</i> -butyl sulfide 19.41					[216]
$\text{C}_8\text{H}_{18}\text{S}$	224	0	108.35	105.9	4.27	23.7
	2*A1 + 6*A2 + A84 1-octanethiol 24.27					[216]
	A1 + 7*A2*B2 + A86					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

<i>T</i> (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_8\text{H}_{19}\text{NSi}$	N-(β -trimethylsilylethyl)trimethylenimine					
199.4	12.9	0	64.68	57.7	12.9	11.5
	A14+A15+A119+3*A1+2*A2+A109					
$\text{C}_8\text{H}_{20}\text{Ge}$	tetraethylgermane					
180.3	12.31	0	68.29	63.7	12.31	11.5
	4*A1+4*A2+A102					
$\text{C}_8\text{H}_{20}\text{O}_4\text{Si}$	tetraethoxysilane					
187.7	13.2	70.32				
191.0	11.14	58.33	128.66	90.6	24.34	17.3
	4*A1+4*A2+4*A32+A109					
$\text{C}_8\text{H}_{20}\text{Pb}$	tetraethyllead					
141.4	9.11	0	64.43	68.7	9.11	9.7
	4*A1+4*A2+A106					
$\text{C}_8\text{H}_{20}\text{Si}$	tetraethylsilane					
189.4	13.01	0	68.72	71.8	13.01	13.6
	4*A1+4*A2+A109					
$\text{C}_8\text{H}_{20}\text{Sn}$	tetraethyltin					
142.1	9.15	0	64.35	74.6	9.15	10.6
	4*A1+4*A2+A110					
$\text{C}_8\text{H}_{24}\text{O}_4\text{Si}_4$	octamethylcyclotetrasiloxane					
258	4.87	18.86				
290.5	23.77	81.81	100.67	58.6	28.63	17.0
	8*A1+A14+5*A15+4*A139+4*A112					
$\text{C}_8\text{H}_{28}\text{N}_4\text{Si}_4$	octamethylcyclotetrasilazane					
367.7	25.05	0	68.13	62.5	25.05	23.0
	8*A1+A14+5*A15+4*A139+4*A121					
$\text{C}_9\text{H}_4\text{Cl}_3\text{NO}_2\text{S}$	2-[(trichloromethyl)thiol]-1H-isoindole-1,3(2H)-dione					
454.2	35.49	0	78.14	74.8	35.49	34.0
	A14+2*A15+A128+2*A19+4*A10+A4*B4+A84+3*A22*E22					
$\text{C}_9\text{H}_4\text{Cl}_4\text{O}_4$	methyl tetrachloroterephthalic acid ester					
444.3	16.89	0	38.01	75.1	16.89	33.4
	4*A2*F22+A38+A36*F36+6*A12+A1					
$\text{C}_9\text{H}_4\text{Cl}_8\text{O}$	1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-isobenzofuran					
395.4	25.94	0	65.61	47.4	25.94	18.7
	3*A14+A15+3*A17+2*A19+4*A16+A112+8*A22*G22					
$\text{C}_9\text{H}_4\text{O}_5$	trimellitic anhydride 1,2,4-benzenetricarboxylic acid					
385	10.46	0	27.18	33.3	10.46	12.8
	A14+2*A15+3*A10+A12+A117+2*A19					
$\text{C}_9\text{H}_5\text{N}_4\text{Cl}_3$	4,6-dichloro-N-(2-chlorophenyl)-1,3,5-triazin-2-amine					
431.0	31.48	0	73.04	68.2	31.48	29.4
	4*A10+5*A12+3*A22*G22+3*A41+A44					
$\text{C}_9\text{H}_6\text{Cl}_2\text{N}_2\text{O}_3$	2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione					
396.3	29.5	0	74.42	63.6	29.5	25.2
	A14+2*A15+A125+2*A22*E22+3*A10+3*A12+A1+A126					
$\text{C}_9\text{H}_6\text{Cl}_6\text{O}_4\text{S}$	6,7,8,9,10,10-hexachloro-6,9-methano-2,4,3-benzodioxathiapin-3,3-dioxide					
419.7	21.66	0	51.6	51.6	21.66	21.7
	3*A14+3*A15+6*A22*D22+3*A17+2*A19+A136+2*A16					
$\text{C}_9\text{H}_6\text{O}_2$	coumarin					
342.1	19.14	0	55.95	48.0	19.14	16.4
	A14+3*A15+A115+A18+A18+A19+A19+4*A10					
$\text{C}_9\text{H}_6\text{O}_2$	chromone					
330.3	17.31	0	52.41	43.3	17.31	14.3
	A14+3*A15+4*A10+A114+A112+2*A18*B18+2*A19					
$\text{C}_9\text{H}_7\text{Cl}_3\text{O}_3$	2-(2,4,5-trichlorophenoxy)propanoic acid					
450.6	39.58	0	87.83	76.0	39.58	34.2
	2*A10+4*A12+3*A22*E22+A36*E36+A32+A3*B3+A1					
$\text{C}_9\text{H}_7\text{Cl}_3\text{O}_3$	methyl 2-(2,4,5-trichlorophenoxy)acetate					
361.9	30.46	0	84.18	70.5	30.46	25.5
	2*A10+4*A12+A2+A32+A38+3*A22*E22+A1					
$\text{C}_9\text{H}_7\text{N}$	quinoline					
220	0.07	0.31				
258.4	10.66	41.27	41.58	47.9	10.73	12.4
	7*A10+2*A12+A41					
$\text{C}_9\text{H}_7\text{N}$	isoquinoline					
299.6	13.54	0	45.21	47.9	13.54	14.3
	7*A10+2*A12+A41					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_9\text{H}_7\text{N}_3\text{S}$	5-methyl-1,2,4-triazolo[3,4- <i>b</i>]benzothiazole 24.07	0	52.3	49.1	24.07	22.6 [221]
C_9H_8	2*A14+2*A15+A1+3*A10+3*A19+A11+A119+2*A118+A131+A18*B18 indene 10.2	0	37.54	42.7	10.2	11.6 [216]
$\text{C}_9\text{H}_8\text{Cl}_2\text{O}_3$	4*A10+2*A15+A14+2*A18+2*A19 methyl 3,6-dichloro-2-methoxybenzoate 18.49	0	60.7	64.8	18.49	19.7 [215]
$\text{C}_9\text{H}_8\text{Cl}_2\text{O}_3$	4*A12+2*A10+2*A1+A38*D38+2*A22*D22+A32 2-(2,4-dichlorophenoxy)propanoic acid 30.43	0	78.18	74.8	30.43	29.1 [215]
$\text{C}_9\text{H}_8\text{Cl}_2\text{O}_3$	3*A10+3*A12+2*A22*D22+A36*D36+A32+A1+A3*B3 methyl 2,4-dichlorophenoxyacetate 25.1	0	79.59	69.3	25.1	21.8 [232]
$\text{C}_9\text{H}_8\text{O}_2$	2*A22*D22+A1+3*A12+3*A10+A38+A32+A2 cinnamic acid 22.63	0	55.71	52.1	22.63	21.2 [215]
$\text{C}_9\text{H}_8\text{O}_2$	5*A10+A12+A6+A36+A6*B6 allocinnamic acid 16.95	0	49.68	52.1	16.95	17.8 [215]
$\text{C}_9\text{H}_9\text{BrO}_3$	5*A10+A12+A6+A36+A6*B6 (<i>dl</i>) 2-(<i>p</i> -bromophenoxy)propanoic acid 31.8	0	82.59	74.9	31.8	28.8 [220]
$\text{C}_9\text{H}_9\text{BrO}_3$	4*A10+2*A12+A1+A3*B3+A36*C36+A21+A32 (<i>d</i>) 2-(<i>p</i> -bromophenoxy)propanoic acid 27.61	0	72.67	74.9	27.61	28.5 [220]
$\text{C}_9\text{H}_9\text{BrO}_3$	4*A10+2*A12+A1+A3*B3+A36*C36+A21+A32 (<i>dl</i>) 3-(<i>m</i> -bromophenyl)-3-hydroxypropanoic acid 26.78	0	76.73	74.6	26.78	26.1 [220]
$\text{C}_9\text{H}_9\text{BrO}_3$	4*A10+A12+A11+C30*A30+A36*C36+A21+A2+A3*B3 (<i>d</i>) 3-(<i>m</i> -bromophenyl)-3-hydroxypropanoic acid 23.85	0	68.14	74.6	23.9	26.1 [220]
$\text{C}_9\text{H}_9\text{BrO}_3$	4*A10+A12+A11+C30*A30+A36*C36+A21+A3*B3+A2 (<i>dl</i>) 3-(<i>p</i> -bromophenyl)-3-hydroxypropanoic acid 28.87	0	77.82	74.6	28.9	27.7 [220]
$\text{C}_9\text{H}_9\text{BrO}_3$	4*A10+A12+A11+A21+C30*A30+A36*C36+A3*B3+A2 (<i>d</i>) 3-(<i>p</i> -bromophenyl)-3-hydroxypropanoic acid 35.56	0	89.36	74.6	35.56	29.7 [220]
$\text{C}_9\text{H}_9\text{ClO}_3$	4*A10+A12+A11+A21+C30*A30+A36*C36+A3*B3+A2 (<i>dl</i>) 2-(<i>o</i> -chlorophenoxy)propanoic acid 32.22	0	83.03	73.4	32.22	28.5 [220]
$\text{C}_9\text{H}_9\text{ClO}_3$	4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32 (<i>d</i>) 2-(<i>o</i> -chlorophenoxy)propanoic acid 26.78	0	72.57	73.4	26.78	27.1 [220]
$\text{C}_9\text{H}_9\text{ClO}_3$	4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32 (<i>dl</i>) 2-(<i>m</i> -chlorophenoxy)propanoic acid 33.05	0	85.63	73.4	33.05	28.3 [220]
$\text{C}_9\text{H}_9\text{ClO}_3$	4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32 (<i>d</i>) 2-(<i>m</i> -chlorophenoxy)propanoic acid 29.71	0	80.83	73.4	29.71	27.0 [220]
$\text{C}_9\text{H}_9\text{ClO}_3$	4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32 (<i>dl</i>) 3-(<i>p</i> -chlorophenyl)-3-hydroxypropanoic acid 29.71	0	83.21	73.1	29.71	26.1 [220]
$\text{C}_9\text{H}_9\text{ClO}_3$	4*A10+A12+A22*C22+C30*A30+A36*C36+A2+A3*B3+A11 (<i>d</i>) 3-(<i>p</i> -chlorophenyl)-3-hydroxypropanoic acid 28.03	0	72.81	73.1	28.03	28.1 [220]
$\text{C}_9\text{H}_9\text{ClO}_3$	4*A10+A12+A11+A22*C22+C30*A30+A36*C36+A3*B3+A2 (<i>dl</i>) 3-(<i>m</i> -chlorophenyl)-3-hydroxypropanoic acid 23.85	0	70.14	73.1	23.85	24.9 [220]
$\text{C}_9\text{H}_9\text{ClO}_3$	4*A10+A12+A11+A22*C22+C30*A30+A36*C36+A2+A3*B3 (<i>d</i>) 3-(<i>m</i> -chlorophenyl)-3-hydroxypropanoic acid 28.03	0	76.18	73.1	28.03	26.9 [220]
$\text{C}_9\text{H}_9\text{ClO}_3$	4*A10+A12+A11+A22*C22+C30*A30+A36*C36+A3*B3+A2 (4-chloro- <i>o</i> -tolylxy)acetic acid 29.98	0	76.3	73.3	29.98	28.8 [215]
$\text{C}_9\text{H}_9\text{ClO}_3$	3*A10+2*A12+A11+A2+A1+A22*C22+A32+A36*C36					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_9\text{H}_9\text{Cl}_2\text{NO}$	3',4'-dichloropropionanilide					
363.7	18.26	0	50.22	58.3	18.26	21.2 [215]
$\text{C}_9\text{H}_9\text{FO}_3$	$A1 + A2 + A60 + 3*A12 + 3*A10 + 2*A22*C22$ (dl) 3-(<i>m</i> -fluorophenyl)-3-hydroxypropanoic acid					
290	20.5	0	70.7	73.5	20.5	21.3 [220]
$\text{C}_9\text{H}_9\text{FO}_3$	$4*A10 + A12 + A11 + A24 + C30*A30 + A36*C36 + A2 + A3*B3$ (d) 3-(<i>m</i> -fluorophenyl)-3-hydroxypropanoic acid					
311	24.27	0	78.03	73.5	24.27	22.9 [220]
$\text{C}_9\text{H}_9\text{FO}_3$	$4*A10 + A12 + A11 + A24 + C30*A30 + A36*C36 + A3*B3 + A2$ (d) 3-(<i>o</i> -fluorophenyl)-3-hydroxypropanoic acid					
342	27.2	0	79.52	73.5	27.2	25.2 [220]
$\text{C}_9\text{H}_9\text{FO}_3$	$4*A10 + A11 + A12 + A24 + C30*A30 + A36*C36 + A2 + A3*B3$ (d) 3-(<i>o</i> -fluorophenyl)-3-hydroxypropanoic acid					
348	22.59	0	64.92	73.5	22.59	25.6 [220]
$\text{C}_9\text{H}_9\text{FO}_3$	$4*A10 + A11 + A12 + A24 + C30*A30 + A36*C36 + A3*B3 + A2$ (dl) 3-(<i>p</i> -fluorophenyl)-3-hydroxypropanoic acid					
362	27.61	0	76.28	73.5	27.61	26.6 [220]
$\text{C}_9\text{H}_9\text{FO}_3$	$4*A10 + A11 + A12 + A24 + C30*A30 + A36*C36 + A2 + A3*B3$ (d) 3-(<i>p</i> -fluorophenyl)-3-hydroxypropanoic acid					
381	30.96	0	81.26	73.5	30.96	28.0 [220]
$\text{C}_9\text{H}_9\text{NO}_4$	$4*A10 + A11 + A12 + A24 + C30*A30 + A36*C36 + A3*B3 + A2$ [(benzoylamino)oxy] acetic acid					
416.9	31.46	0	75.46	72.9	31.46	30.4 [215]
$\text{C}_9\text{H}_9\text{NO}_5$	$5*A10 + A12 + A60 + A32 + A2 + A36*C36$ (dl) 2-(<i>p</i> -nitrophenoxy)propanoic acid					
411.4	32.22	0	78.31	74.9	32.22	30.8 [220]
$\text{C}_9\text{H}_9\text{NO}_5$	$4*A10 + 2*A12 + A1 + A3*B3 + A36*C36 + A32 + A50$ (d) 2-(<i>p</i> -nitrophenoxy)propanoic acid					
362	20.92	0	57.79	74.9	20.92	27.1 [220]
C_9H_{10}	$4*A10 + 2*A12 + A1 + A3*B3 + A36*C36 + A32 + A50$ indane					
221.8	8.6	0	38.77	45.9	8.6	10.2 [216]
C_9H_{10}	$4*A10 + 2*A19 + A14 + 2*A15$ α -methylstyrene					
250.8	11.92	0	47.55	53.8	11.92	13.5 [216]
$\text{C}_9\text{H}_{10}\text{Cl}_2\text{N}_2\text{O}$	$5*A10 + A12 + A1 + A5 + A7$ 3-(3,4-dichlorophenyl)-1,1-dimethylurea					
429.7	33.89	0	78.87	64.8	33.89	27.84 [232]
$\text{C}_9\text{H}_{10}\text{BrClN}_2\text{O}_2$	$2*A1 + 2*A22*C22 + 3*A12 + 3*A10 + A64*B64$ 3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea					
369.8	26.54	0	71.79	68.7	26.54	25.4 [221]
$\text{C}_9\text{H}_{10}\text{Cl}_2\text{N}_2\text{O}_2$	$2*A1 + 3*A10 + 3*A12 + A32 + A22*D22 + A21 + A64$ N' -(3,4-dichlorophenyl)- N -methoxy- N -methylurea					
365.8	26.56	0	72.61	67.3	26.56	24.6 [215]
$\text{C}_9\text{H}_{10}\text{O}$	$2*A22*D22 + A32 + A64 + 2*A1 + 3*A12 + 3*A10$ chroman					
269.8	16.26	0	60.24	50.8	16.26	13.7 [216]
$\text{C}_9\text{H}_{10}\text{O}$	$A14 + 3*A15 + A19 + A19 + A112 + 4*A10$ isochroman					
277.5	16.75	0	60.35	50.8	16.75	14.1 [216]
$\text{C}_9\text{H}_{10}\text{O}$	$A14 + 3*A15 + 2*A19 + A112 + 4*A10$ cinnamyl alcohol					
308.2	15.73	0	51.04	49.0	15.73	15.1 [220]
$\text{C}_9\text{H}_{10}\text{O}$	$5*A10 + A12 + 2*A6 + A2 + A30$ 4-ethylbenzoic acid					
386.2	14.06	0	36.4	50.7	14.06	19.6 [220]
$\text{C}_9\text{H}_{10}\text{O}_2$	$4*A10 + A11 + A12 + A1 + A2 + A36$ hydrocinnamic acid					
321.2	17.68	0	55.04	55.1	17.68	17.7 [215]
$\text{C}_9\text{H}_{10}\text{O}_2$	$5*A10 + A11 + 2*A2 + A36$ phenyl glycidyl ether					
279.8	17.32	0	61.9	61.3	17.32	17.2 [135]
$\text{C}_9\text{H}_{10}\text{O}_2\text{S}$	$A14 + A112 + A32*B32 + 16 + A2 + 5*A10 + A12$ tolyl vinyl sulfone					
340.4	10.88	0	31.96	53.0	10.88	18.0 [238]
	$4*A10 + A11 + A1 + A5 + A6 + A88 + A12$					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
$\text{C}_9\text{H}_{10}\text{O}_3$ 366	(dl) 3-phenyl-3-hydroxypropanoic acid 29.71	0	81.17	59.2	29.71	21.7
	$5*A10+A11+A2+A3*B3+B30*A30+A36*B36$					[220]
$\text{C}_9\text{H}_{10}\text{O}_3$ 391	(d) 3-phenyl-3-hydroxypropanoic acid 32.64	0	83.47	59.2	32.64	23.1
	$5*A10+A11+A2+A3*B3+A30*B30*B36+A36*A36$					[220]
$\text{C}_9\text{H}_{10}\text{O}_3$ 388	(dl) 2-phenoxypropionic acid 33.05	0	85.19	58.2	33.05	22.6
	$5*A10+A12+A1+A3*B3+A36*B36+A32*B32$					[220]
$\text{C}_9\text{H}_{10}\text{O}_3$ 359	(d) 2-phenoxypropionic acid 22.59	0	62.93	58.2	22.59	20.9
	$5*A10+A12+A1+A3*B3+A36*B36+A32*B32$					[220]
$\text{C}_9\text{H}_{10}\text{O}_3$ 358.1	4-methoxyphenylacetic acid 21.8	0	60.88	58.1	21.8	20.8
	$4*A10+A11+A12+A1+A2+A36*B36+A32*B32$					[215]
$\text{C}_9\text{H}_{10}\text{O}_3$ 402.5	4-hydroxyphenylpropionic acid 28.9	0	71.8	63.2	28.9	25.5
	$4*A10+A11+A12+2*A2+A36*B36+A31$					[215]
$\text{C}_9\text{H}_{10}\text{O}_3$ 472.8	4-ethoxybenzoic acid 29.4	0	62.18	60.2	29.4	28.5
	$4*A10+2*A12+A1+A2+A36*B36+A32*B32$					[215]
$\text{C}_9\text{H}_{10}\text{O}_4$ 395	(dl) erythro phenylglyceric acid 31.38	0	79.44	71.9	31.38	28.4
	$5*A10+A11+2*A3*B3+2*C30*A30+A36*C36$					[220]
$\text{C}_9\text{H}_{10}\text{O}_4$ 371.5	(d) erythro phenylglyceric acid 23.43	0	63.07	71.9	23.43	26.7
	$5*A10+A11+2*A3*B3+2*C30*A30+A36*C36$					[220]
$\text{C}_9\text{H}_{11}\text{BrN}_2\text{O}$ 368.3	N'-(4-bromophenyl)-N-methoxy-N-methyl urea 24.44	0	66.36	67.4	24.44	24.8
	$2*A1+A32*C32+4*A10+2*A12+A64*C64+A21$					[215]
$\text{C}_9\text{H}_{11}\text{ClN}_2\text{O}_2$ 353.4	N'-(4-chlorophenyl)-N-methoxy-N-methyl urea 22.54	0	63.78	66.0	22.54	23.3
	$2*A1+4*A10+2*A12+A22*C22+A64*C64+A32$					[215]
$\text{C}_9\text{H}_{11}\text{ClN}_2\text{O}$ 447.6	3-(4-chlorophenyl)-1,1-dimethyl urea 29.46	0	65.82	66.0	29.46	29.6
	$2*A1+A64*B64+A22*B22+2*A12+4*A10$					[215]
$\text{C}_9\text{H}_{11}\text{ClO}_3$ 366.2	2-(4-chloro-2-methylphenoxy)propanoic acid 26.43	0	72.16	73.9	26.43	27.1
	$3*A10+2*A12+A11+A22*C22+A36*C36+A32*C32+A3*B3+2*A1$					[221]
$\text{C}_9\text{H}_{11}\text{Cl}_3\text{NO}_3\text{PS}$ 315	O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate 24.53	0	77.86	87.5	24.53	27.6
	$4*A12+A10+A41+3*A22*E22+2*A1+2*A2+A79$					[215]
$\text{C}_9\text{H}_{11}\text{N}$ 290	1,2,3,4-tetrahydroquinoline 11.81	0	40.73	51.8	11.81	15.0
	$A14+3*A15+A121+A19+4*A10+A19$					[215]
$\text{C}_9\text{H}_{11}\text{N}$ 222.7	5,6,7,8-tetrahydroquinoline 9.08	0	40.75	53.1	9.08	11.8
	$A14+3*A15+3*A10+A41+A19+A19$					[215]
$\text{C}_9\text{H}_{11}\text{NO}_2$ 326	ethyl phenyl carbamate 16.27	0	49.79	64.9	16.27	21.2
	$5*A10+A12+A1+A2+A69$					[102]
$\text{C}_9\text{H}_{11}\text{NO}_2$ 362.8	ethyl 4-aminobenzoate 23.56	0	64.94	68.5	23.56	24.8
	$4*A10+2*A12+A1+A2+A38+A5$					[215,395]
$\text{C}_9\text{H}_{11}\text{NO}_2$ 400.3	p-methoxyacetanilide 27.82	0	69.51	56.0	27.82	22.4
	$2*A1+4*A10+2*A12+A32+A60$					[239]
C_9H_{12} 218.7	1,2,3-trimethylbenzene 0.66	3				
		5.8				
C_9H_{12} 230.3		33.01	41.81	46.2	10.17	11.4
	$3*A1+3*A10+3*A11$					[216]
C_9H_{12} 247.8						
C_9H_{12} 229.3	1,2,4-trimethylbenzene 13.19	0	57.53	46.2	13.19	10.59
	$3*A1+3*A10+3*A11$					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C_9H_{12}	1,3,5-trimethylbenzene					
228.4	9.51	0	41.66	46.2	9.51	10.6
	$3^*A1 + 3^*A10 + 3^*A11$					[216,3]
C_9H_{12}	isopropylbenzene					
177.1	7.32	0	41.34	46.3	7.32	8.2
	$2^*A1 + 5^*A10 + A3 + A11$					[92]
C_9H_{12}	<i>n</i> -propylbenzene					
173.6	9.27	0	53.39	59.3	9.27	10.3
	$5^*A10 + A1 + 2^*A2 + A11$					[215]
$\text{C}_9\text{H}_{12}\text{ClN}_5$	6-chloro- <i>N</i> -cyclopropyl- <i>N'</i> -(1-methylethyl)-1,3,5-triazine-2,4-diamine					
441.6	28.76	0	65.13	60.0	28.76	26.5
	$A14 + A16 + 2^*A1 + A3^*B3 + A22^*F22 + 3^*A41 + 3^*A12 + 2^*A44$					[221]
$\text{C}_9\text{H}_{12}\text{N}_2\text{O}$	1,1-dimethyl-3-phenylurea					
404.8	22.81	0	56.35	64.9	22.81	26.3
	$2^*A1 + 5^*A10 + A12 + A64$					[215]
$\text{C}_9\text{H}_{12}\text{N}_4\text{O}_2$	8-ethyltheophylline					
545.3	37.2	0	68.22	60.2	37.2	32.8
	$2^*A14 + 3^*A15 + 2^*A125 + A118 + A121 + 3^*A1 + 3^*A19 + A2$					[236]
$\text{C}_9\text{H}_{13}\text{BrN}_2\text{O}_2$	5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1 <i>H</i> ,3 <i>H</i>)-pyrimidinedione					
428.3	22.02	0	51.41	68.5	22.02	29.3
	$A14 + 3^*A15 + A124 + A125 + 3^*A1 + A2 + A3^*B3 + A21 + 2^*A19$					[215]
$\text{C}_9\text{H}_{13}\text{ClN}_6$	2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2methylpropanenitrile					
437.9	41.96	0	95.81	70.6	41.96	30.9
	$3^*A41 + A22 + 2^*A44 + 3^*A1 + A2 + A4^*B4 + A56 + 3^*A12$					[215]
$\text{C}_9\text{H}_{13}\text{N}_5$	6,9-dimethyl-8-ethyladenine					
436.8	29.8	0	68.22	61.5	29.8	26.9
	$A14 + 2^*A15 + 3^*A19 + 3^*A1 + A118 + A119 + 2^*A41 + A10 + A12 + A44 + A2$					[240]
$\text{C}_9\text{H}_{14}\text{ClN}_5$	2-chloro-4,6-bis(isopropylamino)-1,3,5-triazine					
490.3	41.87	0	85.39	66.9	41.87	32.8
	$A22^*F22 + 2^*A44 + 3^*A41 + 3^*A12 + 4^*A1 + 2^*A3^*B3$					[215]
$\text{C}_9\text{H}_{14}\text{O}_6$	glyceryl triacetate					
275.3	25.8	0	93.73	80.2	25.8	22.1
	$2^*A2 + 3^*A1 + A3^*B3 + 3^*A38$					[216]
$\text{C}_9\text{H}_{15}\text{N}_3\text{O}_8$	neopentyl-4,4,4-trinitrobutyrate					
333.5	22.59	0	67.75	77.3	22.59	25.8
	$3^*A1 + 3^*A2 + A4 + A4^*B4 + 3^*A50 + A38$					[122]
C_9H_{16}	<i>trans</i> -hexahydroindane					
213.9	10.9	0	50.98	48.4	10.9	10.4
	$2^*A14 + 3^*A15 + 2^*A16$					[184]
C_9H_{16}	<i>cis</i> -hexahydroindane					
182.3	8.26	45.33				
184.5	0.39	2.13				
236.5	1.4	5.91	53.37	48.4	10.05	11.5
	$2^*A14 + 3^*A15 + 2^*A16$					[184]
$\text{C}_9\text{H}_{16}\text{ClN}_5$	6-chloro- <i>N</i> -(1,1-dimethylethyl)- <i>N'</i> -ethyl-1,3,5-triazine-2,4-diamine					
448.6	33.57	0	74.84	70.5	33.57	31.6
	$4^*A1 + A2 + A4^*B4 + 2^*A44 + A22^*F22 + 3^*A41 + 3^*A12$					[221]
$\text{C}_9\text{H}_{16}\text{N}_4\text{OS}$	<i>N</i> -[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]- <i>N,N'</i> -dimethylurea					
435.3	29.48	0	67.72	68.5	29.48	29.8
	$5^*A1 + A4 + A14 + 2^*A15 + A131 + 2^*A118 + 2^*A19 + A64$					[215]
$\text{C}_9\text{H}_{16}\text{O}_4$	azelaic acid					
380	32.67	0	85.97	97.5	32.67	37.1
	$2^*A36^*B36 + 7^*A2^*B2$					[215]
$\text{C}_9\text{H}_{17}\text{N}$	<i>trans</i> -(<i>R,S</i>)-decahydroquinoline					
321.4	25.72	0	80.02	54.3	25.72	17.5
	$2^*A14 + 4^*A15 + A16 + A16 + A121$					[215]
C_9H_{18}	1-nonene					
191.6	19.37	0	104.23	96.1	19.97	18.4
	$A1 + 6^*A2^*B2 + A5 + A6$					[165]
C_9H_{18}	<i>n</i> -butylcyclopentane					
165.2	11.31	0	68.49	65.0	11.31	10.7
	$A14 + A16 + 3^*A2 + 2^*A15$					[216]
C_9H_{18}	<i>n</i> -propylcyclohexane					
178.3	10.37	0	58.19	61.6	10.37	11.0
	$A14 + A1 + A16 + 2^*A2 + 3^*A15$					[215]
$\text{C}_9\text{H}_{18}\text{N}_2\text{O}_2\text{S}$	3,3-dimethyl-1-(methylthio)-2-butanone O-methylcarbamoyloxime					
330.2	19.83	0	60.04	60.4	19.83	20.0

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_9H_{18}N_6$	444.4	23.01	0	51.78	23.01	21.8
						[215]
$C_9H_{18}N_6$	333	16.74	0	50.27	16.74	18.5
						[215]
$C_9H_{18}O$	253.9	29.6	0	116.6	29.6	26.5
						[43]
$C_9H_{18}O$	269.3	24.94	92.59			
	451.8	11.27	24.94	117.5	36.2	37.3
						[215]
$C_9H_{18}O_2$	268	5.61	20.92			
	285.5	20.31	71.13	92.05	25.91	27.5
						[215]
C_9H_{20}	217.2	6.28	28.91			
	219.7	15.48	70.29	99.2	21.76	22.1
						[215, 216]
C_9H_{20}	174.5	7.33	42.0			
	263.4	2.33	8.9	50.9	9.66	11.3
						[216]
C_9H_{20}	206.7	9.75	0	47.17	9.75	8.9
						[216]
C_9H_{20}	208.3	0.48	2.32			
	210.4	0.81	3.85			
	240.1	10.09	42.02	48.2	11.38	15.4
						[216]
$C_9H_{20}N_2O$	311.5	11.1	35.63			
	346.9	14.87	42.87	78.5	25.97	27.6
						[216]
$C_9H_{20}N_2O$	253	20.55	0	81.23	20.55	20.1
						[169, 124]
$C_9H_{20}O$	263	1.9	7.22			
	322	7.3	22.67	29.9	9.2	6.8
						[216]
$C_9H_{20}O_2$	319.6	36.4	0	113.89	36.4	38.4
						[215]
$C_9H_{20}O_2S$	290.8	48.5	0	166.78	48.5	31.8
						[217]
$C_9H_{20}O_3$	272.9	10.2	0	37.38	10.2	30.6
						[243]
$C_9H_{20}S$	267.7	33.5	0	125.14	33.5	30.9
						[136]
$C_9H_{24}Si_2$	223.7	16.05	0	71.75	16.05	16.3
						[216]
$C_9H_{24}Si_3$	269.3	16.5	0	61.26	16.5	12.4
						[216]
$C_{10}F_{14}$	200	0.75	3.77			
	233	1.11	4.77			
	264	10.47	39.66	49.2	12.34	12.9
						[216]
$C_{10}F_{18}$						

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}S_{\text{tpce}}}$ (expt)	$\Delta_0^{T_{\text{fus}}S_{\text{tpce}}}$ (calcd)	$\Delta_0^{T_{\text{fus}}H_{\text{tpce}}}$ (expt)	$\Delta_0^{T_{\text{fus}}H_{\text{tpce}}}$ (calcd)
232.5	4.24	18.2				
266.7	10.3	38.62	56.82	50.3	14.54	13.4
$\text{C}_{10}\text{F}_{18}$	2*A14+4*A15+10*A17+18*A28 <i>trans</i> -perfluorodecalin	0	60.96	50.3	17.96	14.8
	2*A14+4*A15+10*A17+18*A28					[216]
$\text{C}_{10}\text{H}_2\text{O}_6$	pyromellitic dianhydride	1,2,5,6-benzenetetracarboxylic acid				
	15.82	0	28.38	51.9	15.82	28.9
$\text{C}_{10}\text{H}_4\text{Cl}_2\text{O}_2$	2*A14+4*A15+4*A19+2*A117+2*A10 2,3-dichloro-1,4-naphthalenedione		60.83	54.7	28.53	25.7
	28.53	0				[216]
$\text{C}_{10}\text{H}_5\text{Cl}_4\text{NO}_2\text{S}$	A14+3*A15+4*A19+2*A114+2*A22*D22+4*A10 3 α ,4,7,7 α -tetrahydro-2-[(1,1,2,2-tetrachloroethyl)thio]-1H-isoindole-1,3(2H)-dione		92.96	81.4	40.22	35.2
	40.22	0				[215]
$\text{C}_{10}\text{H}_5\text{Cl}_7$	A14+2*A15+2*A19+A128+4*A10+A4*B4+A3*B3+4*A22+A84 1,4,5,6,7,8,8-heptachloro-3 α ,4,7,7 α -tetrahydro-4,7-endo-methanoindene					
	23.4	65.33				
$\text{C}_{10}\text{H}_5\text{Cl}_7\text{O}$	3*A14+A15+3*A17+2*A19+7*A22*G22+2*A18+3*A116 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3 α ,4,7,7 α -tetrahydro-4,7-endo-methanoindan		70.96	41.5	25.49	15.4
	2.09	5.63				[222]
$\text{C}_{10}\text{H}_6\text{Cl}_8$	4*A14-A15+3*A17+2*A19+7*A22*G22+5*A16+A112 1,2,4,5,6,7,8,8-octachloro-2,3,3 α ,4,7,7 α -hexahydro-4,7-methano-1H-indene		55.62	42.4	21.75	18.5
	2.85	6.55				[222]
$\text{C}_{10}\text{H}_6\text{Cl}_4\text{O}_4$	3*A14+A15+3*A17+2*A19+2*A16+8*A22*G22 dimethyl-2,3,5,6-tetrachloro-1,4-benzenedicarboxylate		60.94	46.1	23.15	17.5
	23.15	0				[221]
$\text{C}_{10}\text{H}_6\text{OS}_2$	6*A12+4*A22*F22+2*A38+2*A1 naphthalene 1,8-disulfide S-oxide		70.01	70.3	30.23	30.4
	30.23	0				[215]
$\text{C}_{10}\text{H}_6\text{S}_2$	A14+2*A15+2*A19+A19+6*A10+A12+A133 naphthalene disulfide					
	3.2	8.8				
$\text{C}_{10}\text{H}_7\text{Br}$	7*A10+3*A12+A21 2-bromonaphthalene	18.09	61.85	47.0	20.17	15.5
	14.40	43.76				[216]
$\text{C}_{10}\text{H}_7\text{Cl}$	7*A10+2*A12+A12+A21 1-chloronaphthalene	0	47.65	40.2	12.9	10.9
	12.9	0				[83]
$\text{C}_{10}\text{H}_7\text{Cl}$	7*A10+3*A12+A22 2-chloronaphthalene		44.28	40.2	14.7	13.4
	14.7	0				[83]
$\text{C}_{10}\text{H}_7\text{Cl}_3\text{O}$	2-(3,5-dichlorophenyl)-2(2,2,2-trichloroethyl)oxirane		59.17	62.9	18.54	19.7
	18.54	0				[221]
$\text{C}_{10}\text{H}_7\text{I}$	A14+2*A12+A11+3*A10+A17+A112+5*A22*F22+A2+A4*B4 1-iodonaphthalene		56.82	48.8	15.91	13.7
	15.91	0				[215]
$\text{C}_{10}\text{H}_7\text{I}$	7*A10+3*A12+A29 2-iodonaphthalene		48.96	48.8	16.04	16.0
	16.04	0				[215]
$\text{C}_{10}\text{H}_7\text{NO}_2$	7*A10+3*A12+A29 1-nitronaphthalene		55.87	47.2	18.43	15.6
	18.43	0				[215]
C_{10}H_8	7*A10+3*A12+A50 naphthalene		53.75	44.4	19.1	15.7
	19.1	0				[215]
C_{10}H_8	8*A10+2*A12 azulene					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)	
373.5	17.53	0	46.9	44.2	17.53	16.5	
$\text{C}_{10}\text{H}_8\text{ClN}_3\text{O}$	2*A14+4*A15+2*A19+8*A18 5-amino-4-chloro-2-phenyl-3(2H)-pyridazinone						[244]
479.2	26.75	0	55.83	62.8	26.75	30.1	
$\text{C}_{10}\text{H}_8\text{ClN}_3\text{O}_2$	A14+3*A15+2*A19+A18*B18+A45+A22*D22+A125 +5*A10+A12+A118 4-(2-chlorophenylhydrazono)-3-methyl-5-isoxazolone						[215]
440.4	28.04	0	63.66	61.3	28.04	27.0	
$\text{C}_{10}\text{H}_8\text{O}$	A14+2*A15+2*A19+A115+A118+A42+A1+4*A10+2*A12+A44+A22*E22 α -naphthol						[221]
369	23.01	0	62.34	49.7	23.01	18.4	
$\text{C}_{10}\text{H}_8\text{O}$	7*A10+2*A12+A31+A12 β -naphthol						[215]
393.6	18.79	0	47.7	49.7	18.79	19.6	
$\text{C}_{10}\text{H}_8\text{O}_3$	7*A10+2*A12+A31+A12 4-methyl-7-hydroxycoumarin						[215]
460.7	29.14	0	63.25	60.3	29.14	27.8	
$\text{C}_{10}\text{H}_9\text{Cl}_2\text{NO}$	A14+3*A15+A115+A31+3*A19+A18*B18+3*A10+A12+A1 N-(3,4-dichlorophenyl)-2-methyl-2-propenamide						[216]
395.5	32.04	0	81.0	57.8	32.04	22.9	
$\text{C}_{10}\text{H}_9\text{Cl}_3\text{O}_3$	A1+A5+A7+3*A10+3*A12+2*A22*C22+A60 methyl 2-(2,4,5-trichlorophenoxy)propionate						[215]
360.6	31.95	0	88.59	71.3	31.95	25.7	
$\text{C}_{10}\text{H}_9\text{Cl}_3\text{O}_3$	2*A10+4*A12+2*A1+A3*B3+A32+A38+3*A22*E22 4-(2,4,5-trichlorophenoxy)butanoic acid						[215]
386.7	30.28	0	78.3	89.6	30.28	34.6	
$\text{C}_{10}\text{H}_9\text{Cl}_4\text{NO}_2\text{S}$	2*A10+4*A12+3*A22*E22+A36*E36+A32+3*A2 N-[(1,1,2,2-tetrachloroethyl)thio]-4-cyclohexene-1,2-dicarboximide						[215]
432	43.1	0	99.76	80.5	43.1	34.8	
$\text{C}_{10}\text{H}_9\text{N}$	2*A14+3*A15+2*A16+2*A18+A128+A4*B4+A3*B3+4*A22*G22+A84 1-naphthylamine						[232]
323.2	15.53	0	48.05	50.8	15.53	16.4	
$\text{C}_{10}\text{H}_9\text{N}$	7*A10+2*A12+A45+A12 2-naphthylamine						[215]
386.2	23.33	0	60.38	50.8	23.33	19.6	
$\text{C}_{10}\text{H}_9\text{NO}_2$	7*A10+2*A12+A45+A12 4-methyl-7-aminocoumarin						[215]
499.9	32.09	0	64.19	61.4	32.09	30.7	
$\text{C}_{10}\text{H}_{10}$	A14+3*A15+A115+A45+3*A19+A18*B18+3*A10+A12+A1 bullvalene						[216]
366.5	15.25	0	41.61	35.3	15.25	12.9	
$\text{C}_{10}\text{H}_{10}\text{Cl}_2\text{O}_3$	3*A14+A15+4*A16+6*A18 4-(2,4-dichlorophenoxy)butyric acid						[216]
391.4	38.42	0	98.16	88.3	38.42	34.6	
$\text{C}_{10}\text{H}_{10}\text{O}_3$	3*A10+3*A12+3*A2+A36*D36+2*A22*D22+A32 2,3-dihydro-2,2-dimethyl-7-benzofuranol-3-one						[215]
440.6	21.79	0	49.47	49.6	21.79	21.9	
$\text{C}_{10}\text{H}_{10}\text{O}_4$	A14+2*A15+2*A19+A17+A112+A114+2*A1+A31+3*A10+A11 1,2-dicarbomethoxybenzene						[221]
274.2	16.95	0	61.92	65.2	16.95	17.9	
$\text{C}_{10}\text{H}_{10}\text{O}_4$	4*A10+2*A38+2*A12+2*A1 1,3-dicarbomethoxybenzene						[217]
341.2	25.3	0	74.15	65.2	25.3	22.3	
$\text{C}_{10}\text{H}_{10}\text{O}_4$	4*A10+2*A38+2*A12+2*A1 1,4-dicarbomethoxybenzene						[217]
413.8	32.09	0	77.55	65.2	32.09	27.0	
$\text{C}_{10}\text{H}_{11}\text{ClO}_3$	4*A10+2*A38+2*A12+2*A1 (dl) 2-(2-chloro-3-methylphenoxy)propionic acid						[217]
391.5	30.54	0	78.02	73.9	30.54	29.0	
$\text{C}_{10}\text{H}_{11}\text{ClO}_3$	3*A10+2*A1+A3*B3+2*A12+A11+A32+A36*C36+A22*C22 (D) 2-(2-chloro-3-methylphenoxy)propionic acid						[273]
359.5	22.18	0	61.68	73.9	22.18	26.6	
$\text{C}_{10}\text{H}_{11}\text{F}_3\text{N}_2\text{O}$	3*A10+2*A1+A3*B3+2*A12+A11+A32+A36*C36+A22*C22 N,N-dimethyl-N'-[3-(trifluoromethyl)-phenyl]urea						[273]
434.1	29.82	0	68.69	65.0	29.82	28.2	
	2*A1+A11+A12+A4*B4+3*A25+4*A10+A64*B64						[215]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{10}H_{11}F_3N_2O_3S$ 455.7	N-[4-methyl-3-[(trifluoromethyl)sulfonyl]amino]phenyl]acetamide 40.47	0	88.81	57.9	40.47	20.4 [221]
$C_{10}H_{11}NO_3$ 408	2*A1+3*A10+A11+2*A12+A4*B4+3*A25+A95+A60 N-salicylidene- β -alanine 28.5	0	69.85	81.4	28.5	33.2 [216]
$C_{10}H_{12}$ 237.4	2*A2+A36*C36+4*A10+2*A12+A31+A6*B6+A42 1,2,3,4-tetrahydronaphthalene 12.45	0	52.44	49.6	12.45	11.8 [216]
$C_{10}H_{12}$ 216	A14+3*A15+4*A10+2*A19 <i>endo</i> -dicyclopentadiene 9.66	44.72				
$C_{10}H_{12}$ 304.8	2.22 3*A14+A15+4*A16+4*A18 isopropyl-3-chlorophenylcarbamate 17.75	7.28	52.01	38.5	11.88	11.7 [216]
$C_{10}H_{12}ClNO_2$ 313.9	2*A1+A3*B3+4*A10+2*A12+A69+A22*B22 5-chloro-6-[[[(methylamino)carbonyl]oxy]imino]bicyclo[2.2.1]heptane-2-carbonitrile 26.07	0	60.4	59.6	26.07	25.7 [221]
$C_{10}H_{12}ClN_3O_2$ 431.6	2*A14+A15+A56+A22*D22+2*A16+2*A16+A19+A42+A69+A1 allobarbitol 32.31	0	73	73.4	32.31	32.5 [241]
$C_{10}H_{12}N_2O_3$ 442.6	A14+3*A15+A129+A124+A17+2*A2+2*A5+2*A6 2-ethoxyisnitrosoacetanilide 23	0	56.79	63.0	23	25.5 [216]
$C_{10}H_{12}N_2O_3$ 405	A1+A2+4*A10+2*A12+A32+A60+A53+A6*B6 4-ethoxyisnitrosoacetanilide 7.6	0	15.51	63.0	7.6	30.9 [216]
$C_{10}H_{12}N_2O_3S$ 412.5	A1+A2+4*A10+2*A12+A32+A60+A53+A6*B6 3-(1-methylethyl)-(1H)-2,1,3-benzothiadiazin-4(3H)-one 2,2-dioxide 21.77	0	52.76	53.0	21.77	21.9 [221]
$C_{10}H_{12}N_2O_5$ 313.7	A14+3*A15+2*A19+A125+4*A10+2*A1+A3*B3+A137 2-sec-butyl-4,6-dinitrophenol 21.81	0	69.54	64.4	21.81	20.2 [221]
$C_{10}H_{12}N_2S$ 375	2*A10+A11+3*A12+2*A1+A2+A3+2*A50+A31 N-allyl-N-phenylthiourea 27.61	0	73.64	73.7	27.61	27.6 [216]
$C_{10}H_{12}N_3O_3PS_2$ 345.3	5*A10+A12+A2+A5+A6+A90 S-(3,4-dihydro-4-oxobenzo[d][1,2,3]-triazin-3-ylmethyl) O,O-dimethylphosphorodithioate 27.76	0	80.4	61.6	27.76	21.3 [215]
$C_{10}H_{12}O_2$ 301	A14+3*A15+2*A118+2*A19+4*A10+A125+A2+2*A1+A80 4-propylbenzoic acid 3.4	11.3				
$C_{10}H_{12}O_2$ 422	23.3 A1+2*A2+A11+A12+4*A10+A36 (dl) 3-hydroxy-3-phenylbutyric acid 19.66	55.21	66.51	57.8	26.7	24.4 [177]
$C_{10}H_{12}O_3$ 330	A1+A2+A4*B4+5*A10+A11+A36*B36+B30*A30 (d) 3-hydroxy-3-phenylbutyric acid 22.59	0	59.59	63.6	19.66	21.0 [220]
$C_{10}H_{12}O_3$ 357	A1+A2+A4*B4+5*A10+A11+B36*A36+B30*A30 (d) 3-hydroxy-3-phenylbutyric acid 22.59	0	63.29	63.6	22.59	22.7 [220]
$C_{10}H_{12}O_3$ 360.2	4-ethoxyphenylacetic acid 23	0	63.85	65.2	23	23.5 [215]
$C_{10}H_{12}O_3$ 376.9	4*A10+A11+A12+2*A2+A1+A36*B36+A32 4-methoxyphenylpropionic acid 28.5	0	75.62	65.2	28.5	24.6 [215]
$C_{10}H_{12}O_3$ 369.2	4*A10+A11+A12+2*A2+A1+A36*B36+A32 propyl 4-hydroxybenzoate 27.99	0	75.82	74.5	27.99	27.5
$C_{10}H_{12}O_3$ 369.8	26.7 A1+2*A2+4*A10+2*A12+A31+A38 N'-(3-chloro-4-methoxyphenyl)-N,N-dimethylurea 27.48	0	72.3	74.5	26.7	27.5 [218, 395]
$C_{10}H_{13}ClN_2O_2$ 399.2	3*A1+3*A10+3*A12+A22*C22+A32+A64*C64 2-((4-chloro-6-(cyclopropylamino)-1,3,5-triazin-2-yl)amino)-2-methylpropanenitrile 22.51	0	51.34	64.6	22.51	28.3 [221]
$C_{10}H_{13}ClN_6$ 438.5	A14+A16+3*A41+3*A12+A22*F22+2*A44+2*A1+A56+A4*B4					28.3 [221]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
$\text{C}_{10}\text{H}_{13}\text{ClO}_3$	4-(4-chloro-2-methylphenoxy)butanoic acid					
373.4	32.02	0	85.73	87.6	32.02	32.7
	$3^*A10 + 2^*A12 + A11 + A22^*C22 + A36^*C36 + A32 + 3^*A2 + A1$					[221]
$\text{C}_{10}\text{H}_{13}\text{NO}_2$	propyl 4-aminobenzoate					
347.1	20.54	64.61	59.18	75.6	20.54	26.2
	$4^*A10 + 2^*A12 + A1 + A45 + A38 + 2^*A2$					[215]
$\text{C}_{10}\text{H}_{13}\text{NO}_2$	methyl <i>p</i> -N,N-dimethylaminobenzoate					
371.8	26.07	0	70.12	52.9	26.07	19.7
	$3^*A1 + A38 + A43 + 4^*A10 + 2^*A12$					[215]
$\text{C}_{10}\text{H}_{13}\text{NO}_2$	<i>p</i> -ethoxyacetanilide					
407.2	31.25	0	76.75	63.1	31.25	25.7
408.6	30.83	0	75.5	63.1	30.8	25.7
	$2^*A1 + 4^*A10 + 2^*A12 + A32 + A60 + A2$					[239, 395]
$\text{C}_{10}\text{H}_{13}\text{NO}_2$	propyl <i>N</i> -phenyl carbamate					
331	21.08	0	63.68	72.0	21.08	23.9
	$2^*A2 + A1 + 5^*A10 + A12 + A69$					[102]
$\text{C}_{10}\text{H}_{13}\text{NO}_2$	isopropyl phenylcarbamate					
359.5	19.37	0	53.88	65.7	19.37	23.62
	$5^*A10 + A12 + 2^*A1 + A3^*B3 + A69$					[215]
$\text{C}_{10}\text{H}_{13}\text{NO}_2$	3,4-dimethylphenyl methylcarbamate					
350.8	24.97	0	71.17	58.9	24.97	20.7
	$3^*A1 + 2^*A11 + A12 + 3^*A10 + A69$					[215]
$\text{C}_{10}\text{H}_{13}\text{NO}_4$	2-(1,3-dioxolan-2-yl)phenyl methylcarbamate					
387.2	23.82	0	61.51	69.3	23.82	26.8
	$A14 + 2^*A15 + A16 + 2^*A112 + 4^*A10 + A11 + A12 + A69 + A1$					[221]
$\text{C}_{10}\text{H}_{13}\text{N}_5\text{O}_3$	2-acetylamino-9-[(2-hydroxyethoxy)methyl]-9H-purine					
454.2	54.92	0	120.9	84.0	54.92	38.2
	$A14 + 2^*A15 + 2^*A19 + A18^*B18 + 2^*A41 + A118 + A119$					[203]
	$+ 3^*A2 + A30^*F30 + A32 + A60 + A1 + A10 + A12$					
$\text{C}_{10}\text{H}_{13}\text{N}_5\text{O}_3$	9-[(2-acetoxyethoxy)methyl]-2-amino-9H-purine					
408.2	42.69	0	104.58	88.9	42.69	36.3
	$A14 + 2^*A15 + 2^*A19 + A18^*B18 + 2^*A41 + A118 + A119 +$					[203]
	$3^*A2 + A32 + A38 + A1 + A10 + A12 + A45$					
$\text{C}_{10}\text{H}_{13}\text{N}_5\text{O}_4$	2-acetylamino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one					
490.2	53.83	0	109.81	90.3	53.83	44.3
	$2^*A14 + 3^*A15 + 3^*A19 + A18^*B18 + 2^*A118 + A119 +$					[203]
	$A124 + A60 + 3^*A2 + A30^*F30 + A32 + A1$					
$\text{C}_{10}\text{H}_{13}\text{N}_5\text{O}_4$	2-amino-9-[(2-acetoxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one					
515.2	49.9	0	96.86	95.1	49.9	49.0
	$2^*A14 + 3^*A15 + 3^*A19 + A18^*B18 + 2^*A118 + A119 +$					[203]
	$A124 + A45 + 3^*A2 + A38 + A32 + A1$					
$\text{C}_{10}\text{H}_{14}$	<i>tert</i> -butylbenzene					
215	8.40	0	39.1	45.4	8.40	9.8
	$3^*A1 + A4 + 5^*A10 + A11$					[216]
$\text{C}_{10}\text{H}_{14}$	1,2,3,4-tetramethylbenzene					
265.4	11.23	0	42.31	46.7	11.23	12.4
	$4^*A1 + 2^*A10 + 4^*A11$					[216]
$\text{C}_{10}\text{H}_{14}$	1,2,3,5-tetramethylbenzene					
248.6	12.93	0	52.01	46.7	12.93	11.6
	$4^*A1 + 2^*A10 + 4^*A11$					[216]
$\text{C}_{10}\text{H}_{14}$	1,2,4,5-tetramethylbenzene					
352.4	20.88	0	59.25	46.7	20.88	16.5
	$4^*A1 + 2^*A10 + 4^*A11$					[216]
$\text{C}_{10}\text{H}_{14}$	1-isopropyl-4-methylbenzene					
204.2	9.67	0	47.33	46.8	9.67	9.6
	$3^*A1 + A3 + 4^*A10 + 2^*A11$					[216]
$\text{C}_{10}\text{H}_{14}$	<i>n</i> -butylbenzene					
185.3	11.22	0	60.56	66.5	11.22	12.3
	$5^*A10 + A1 + 3^*A2 + A11$					[216]
$\text{C}_{10}\text{H}_{14}\text{Cl}_2\text{NO}_2\text{PS}$	O-(2,4-dichlorophenyl) O-methyl-(1-methylethyl) phosphoramidothioate					
321.5	29.25	0	90.99	91.1	29.25	29.3
	$3^*A10 + 3^*A12 + 3^*A1 + A3^*B3 + A82 + 2^*A22^*C22$					[221]
$\text{C}_{10}\text{H}_{14}\text{NO}_5\text{PS}$	O,O-diethyl O-4-nitrophenyl phosphorothioate					
278.1	15.72	0	56.55	83.0	15.72	23.1
	$4^*A10 + 2^*A12 + 2^*A1 + 2^*A2 + A50 + A79$					[215]
$\text{C}_{10}\text{H}_{14}\text{N}_4\text{O}_2$	8-propyltheophylline					
534.3	33.3	0	62.32	67.3	33.3	36.0
	$2^*A14 + 3^*A15 + 2^*A125 + A118 + A121 + 3^*A1 + 3^*A19 + 2^*A2$					[215]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_{10}\text{H}_{14}\text{N}_4\text{O}_2$	8-isopropyltheophylline					
569.3	34.4	0	60.43	54.3	34.4	30.9
	$2^*A14+3^*A15+2^*A125+A118+A121+2^*A1+3^*A19+2^*A1+A3$					[215]
$\text{C}_{10}\text{H}_{14}\text{N}_6\text{O}$	1-(2-hydroxyethylmethylamino)-3,5-bis(dimethylamino)-s-triazine					
373.3	17.32	0	46.4	68.5	17.32	25.6
	$5^*A1+2^*A2+A30^*F30+3^*A43+3^*A41+3^*A12$					[242]
$\text{C}_{10}\text{H}_{14}\text{O}$	4- <i>tert</i> -butylphenol					
373.2	14.52	0	38.9	50.7	14.52	18.9
	$3^*A1+A4+4^*A10+A11+A12+A31$					[101]
$\text{C}_{10}\text{H}_{14}\text{O}$	thymol					
324.2	22.01	0	67.88	52.2	22.01	16.9
	$3^*A10+2^*A11+A12+3^*A1+A3+A31$					[220]
$\text{C}_{10}\text{H}_{14}\text{O}_2$	4-propylbenzoic acid					
301	3.4	11.3				
422	23.3	55.21	66.51	57.8	26.7	24.4
	$A1+2^*A2+4^*A10+A11+A12+A36$					[177]
$\text{C}_{10}\text{H}_{14}\text{O}_3$	D-camphoric anhydride					
406	29	71.43				
495	8.7	17.58	89	45.3	37.7	22.4
	$2^*A14+2^*A15+A17+A17+A16+3^*A1+A117$					[45]
$\text{C}_{10}\text{H}_{14}\text{O}_3$	DL-camphoric anhydride					
375	24	64				
495	8.7	17.58	81.58	45.3	32.7	17.0
	$2^*A14+2^*A15+A17+A17+A16+3^*A1+A117$					[45]
$\text{C}_{10}\text{H}_{14}\text{O}_8$	(<i>dl</i>) dimethyl diacetyltartrate					
355.2	25.94	0	73.03	81.4	25.94	28.9
	$4^*A1+2^*A3^*B3+4^*A38$					[226]
$\text{C}_{10}\text{H}_{14}\text{O}_8$	(<i>d</i>) dimethyl diacetyltartrate					
377.2	29.29	0	77.65	81.4	29.29	30.7
	$4^*A1+2^*A3^*B3+4^*A38$					[226]
$\text{C}_{10}\text{H}_{14}\text{Si}$	1-phenyl-1-methyl-1-silacyclobutane					
210.1	12.28	0	58.45	47.5	12.28	10.0
	$5^*A10+A11+A14+A15+A139+A1$					[216]
$\text{C}_{10}\text{H}_{14}\text{Si}$	vinyl dimethylphenylsilane					
190.7	12.26	0	64.28	58.9	12.26	11.2
	$2^*A1+A5+A6^*B6+5^*A10+A12+A109$					[216]
$\text{C}_{10}\text{H}_{15}\text{Br}$	1-bromoadamantane					
279	0.88	3.15				
310.5	6.93	22.32				
396.5	3.83	9.66	35.13	42.6	11.64	16.9
	$3^*A14+A15+3^*A16+A17+A21$					[146]
$\text{C}_{10}\text{H}_{15}\text{Cl}$	1-chloroadamantane					
244.2	6.01	24.61				
442.5	4.87	11.01	35.62	35.9	10.88	15.9
	$3^*A14+A15+3^*A16+A17+A22$					[146]
$\text{C}_{10}\text{H}_{15}\text{I}$	1-iodoadamantane					
211	2.14	10.7				
347	10.22	51.1	61.8	44.5	12.36	15.4
	$3^*A14+A15+3^*A16+A17+A29$					[146]
$\text{C}_{10}\text{H}_{15}\text{N}_5$	6,9-dimethyl-8-propyladenine					
411.9	30.2	0	73.32	68.7	30.2	28.3
	$A14+2^*A15+3^*A19+3^*A1+A118+A119+2^*A41+A10+A12+A44+2^*A2$					[240]
$\text{C}_{10}\text{H}_{15}\text{NO}$	(L) carvoxime					
346.5	22.72	0	65.57	58.9	22.72	20.4
	$A14+3^*A15+2^*A1+A16+A19+A18+A19+A5+A7+A53$					[226]
$\text{C}_{10}\text{H}_{15}\text{NO}$	(DL) carvoxime					
365.1	17.03	0	46.64	58.9	17.03	21.5
	$A14+3^*A15+2^*A1+A16+A19+A18+A19+A5+A7+A53$					[226]
$\text{C}_{10}\text{H}_{16}$	tricyclo[5.2.1.0 ^{2,6}]decane					
352	2.95	0	8.38	0	2.95	0
	No prediction made					[216]
$\text{C}_{10}\text{H}_{16}$	adamantane					
208.6	3.38	16.18				
541.2	10.9	20.14	36.32	44.9	14.28	24.3
	$3^*A14+A15+4^*A16$					[216, 189, 192]
$\text{C}_{10}\text{H}_{16}\text{Cl}_3\text{NOS}$	S-2,3,3-trichloroallyl diisopropylthiocarbamate					
306	27.11	0	88.48	88.6	27.11	27.1

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)	
$C_{10}H_{16}NO_4PS$	$A5 + A7 + A4 * B4 + 4 * A1 + 2 * A3 * B3 + 3 * A22 * C22 + A93$ O-[4-(dimethylamino)sulfonyl]phenyl] O,O-dimethyl phosphorothionate	26.5	0	81.08	74.8	26.5	[215]
326.8							
$C_{10}H_{16}N_2$	$A94 + 4 * A1 + A79 + 4 * A10 + 2 * A12$ ethyl(1,1-dimethylpropyl)malononitrile	19.25	0	62.59	62.4	19.25	[221]
307.5							
$C_{10}H_{16}N_4O_2S$	$4 * A1 + 2 * A2 + A4 + A4 * B4 + 2 * A56$ 3-(5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl)-4-hydroxy-1-methyl-2-imidazolidinone	25.46	0	62.26	62.2	25.46	[245]
408.9							
$C_{10}H_{16}O$	$2 * A14 + 4 * A15 + A127 + A16 + 4 * A1 + A4 + 2 * A19 + A131 + 2 * A118 + A30 * E30$ (D) camphor	16.0	66.1				
242		0.23	0.62				
374		5.3	11.7	78.5	38.0	21.5	17.2
452							[45]
$C_{10}H_{16}O_2$	$A114 + 2 * A14 + A15 + A17 + A17 + A16 + 3 * A1$ 1,6-cyclodecanedione	29.58	0	79.5	56.6	29.58	21.1
372.2							[114]
$C_{10}H_{16}O_4$	$A14 + 7 * A15 + 2 * A114$ 1,4-cyclohexanedione bis ethylene ketal	25.77	0	72.97	54.4	25.77	19.2
353.2							[114]
$C_{10}H_{17}NO$	$3 * A14 + 5 * A15 + 4 * A112 + 2 * A17$ D camphor oxime	13.3	34.73				
383		1.8	4.63	39.35	40.6	15.1	15.8
389							[45]
$C_{10}H_{17}NO$	$2 * A14 + A15 + A16 + A17 + A17 + 3 * A1 + A53 + A19$ DL camphor oxime	3	8				
375		11.2	29.47				
380		1.2	3.09	40.57	40.6	15.4	15.8
388							[45]
$C_{10}H_{17}N_5O$	$2 * A14 + A15 + A16 + A17 + A17 + 3 * A1 + A53 + A19$ 6-methoxy-N,N'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine	21.18	0	58.26	73.0	21.18	26.5
363.5							[215]
$C_{10}H_{18}$	$5 * A1 + 2 * A3 * B3 + A32 + 3 * A41 + 3 * A12 + 2 * A44$ <i>cis</i> -decalin	14.43	0	59.45	52.1	14.43	12.65
242.8							[216]
$C_{10}H_{18}$	$2 * A14 + 4 * A15 + 2 * A16$ <i>trans</i> -decalin	2.13	9.87				
216.1		9.49	41.22	51.1	52.1	11.62	11.99
230.2							[216]
$C_{10}H_{18}N_5S$	$2 * A14 + 4 * A15 + 2 * A16$ N-(1,1-dimethylethyl)-N'-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine	21.42	0	56.99	74.0	21.42	27.8
375.9							[221]
$C_{10}H_{18}N_6O_2$	$5 * A1 + A2 + A4 * B4 + 2 * A44 + 3 * A41 + 3 * A12 + A84$ 1-(sarcosine)-3,5-bis(dimethylamino)-s-triazine	29.83	0	69.33	68.6	29.83	29.6
431							[242]
$C_{10}H_{18}O_4$	$5 * A1 + 3 * A41 + 3 * A12 + 3 * A43 + A36 * F36 + A2$ sebacic acid	40.8	0	101.0	106.9	40.8	43.2
404							[216]
$C_{10}H_{18}Si$	$8 * A2 * B2 + 2 * A36 * B36$ 5-trimethylsilyl-2-norbornene	6.84	0	33.93	78.4	6.84	15.81
201.6							[162]
$C_{10}H_{20}$	$2 * A14 + A14 + 3 * A16 + 2 * A18 + 3 * A1 + A109$ <i>n</i> -butylcyclohexane	14.14	0	71.28	68.7	14.14	13.6
198.4							[216]
$C_{10}H_{20}$	$A14 + A1 + A16 + 3 * A2 + 3 * A15$ 1-decene	7.95	40.09				
198.3		13.81	66.73	106.8	105.5	21.76	21.8
206.9							[216]
$C_{10}H_{20}$	$A1 + 7 * A2 * B2 + A5 + A6$ 2,2,5,5-tetramethylhex-3-ene	1.21	5.13				
235.8		4.33	17.78				
243.5		10.25	38.12	61.03	46.3	15.79	12.5
268.9							[42]
$C_{10}H_{20}N_6$	$6 * A1 + 2 * A4 + 2 * A6$ 1-(ethylmethylamino)-3,5-bis(dimethylamino)-s-triazine	21.3	0	55.46	56.3	21.3	21.6
384							[215]
$C_{10}H_{20}O$	$3 * A41 + 3 * A12 + 2 * A43 + 6 * A1 + A44 + A3 * B3$ (<i>dl</i>) menthol						

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (calcd)
301.2	10.25	0	34.03	38.4	10.25	11.6
$C_{10}H_{20}O$	$3*A1 + A14 + 3*A15 + 2*A16 + A30 + A3 + A16$ (<i>l</i>) menthol					[226]
	11.88	0	37.58	38.4	11.88	12.1
$C_{10}H_{20}O$	$3*A1 + A14 + 3*A15 + 2*A16 + A30 + A3 + A16$ decanal					[226]
	30.6	0	114.1	113.8	30.6	30.5
$C_{10}H_{20}O_2$	$8*A2*B2 + A1 + A34$ decanoic acid					[93]
	27.99	0	91.28	105.6	27.82	32.2
$C_{10}H_{22}$	$8*A2*B2 + A1 + A36$ <i>n</i> -decane					[216]
	28.7	0	117.99	109.8	28.7	26.7
$C_{10}H_{22}$	$2*A1 + 8*A2*B2$ 5-methylnonane					[216]
	16.65	0	89.19	79.2	16.65	14.8
$C_{10}H_{22}$	$3*A1 + 6*A2 + A3$ (DL) 4-methylnonane					[216]
	15.19	0	86.94	79.2	15.19	13.8
$C_{10}H_{22}$	$3*A1 + 6*A2 + A3$ (DL) 3-methylnonane					[216]
	18.7	0	99.22	92.4	18.7	17.4
$C_{10}H_{22}$	$3*A1 + 6*A2*B2 + A3$ 2-methylnonane					[216]
	17.49	0	87.97	92.4	17.49	18.4
$C_{10}H_{22}O_2$	$3*A1 + 6*A2*B2 + A3$ 1,10-decanediol					[216]
	41.7	0	120.69	129.5	41.7	44.8
$C_{10}H_{22}O_2S$	$10*A2*B2 + 2*A30*B30$ 3(<i>n</i> -heptylthio)-1,2-propanediol					[215]
	27.3	94.3				
$C_{10}H_{22}O_3$	1.7	5.81	100.11	114.3	29.0	33.4
	$A1 + 6*A2*B2 + A84 + 2*A30*C30 + A3*B3 + 2*A2$ 3(<i>n</i> -heptyloxy)-1,2-propanediol					[217]
$C_{10}H_{22}O_3$	28.8	100				
	1	4.06	104.06	116.9	29.8	28.8
$C_{10}H_{22}S$	$A1 + 6*A2*B2 + A32 + 2*A30*C30 + A3*B3 + 2*A2$ 1-decanethiol					[217]
	33.3	0	134.31	124.6	33.3	30.9
$C_{10}H_{23}NO_2$	$9*A2*B2 + A1 + A86$ 3(<i>n</i> -heptylamino)-1,2-propanediol					[216]
	28.8	0	88.64	106.9	28.8	34.7
$C_{10}H_{26}O_3Si_3$	$A1 + 6*A2*B2 + A44 + 2*A30*C30 + A3*B3 + 2*A2$ 1,1,3,3-tetraethyl-5,5-dimethylcyclotrisiloxane					[217]
	0.13	0.67				
$C_{11}H_8O_2$	9.52	36.62	37.29	78.1	9.65	20.3
	$6*A1 + 4*A2 + 3*A112 + 3*A139 + A14 + 3*A15$ 1-naphthoic acid					[216]
$C_{11}H_8O_2$	19.89	0	45.7	42.8	19.89	18.6
	$7*A10 + 2*A12 + A36 + A12$ 2-naphthoic acid					[215]
$C_{11}H_8O_2$	23.54	0	51.15	42.8	23.54	19.7
	$7*A10 + 2*A12 + A36 + A12$ 4-chlorobut-2-ynyl 3-chlorophenylcarbamate					[215]
$C_{11}H_9Cl_2NO_2$	26.91	0	78.21	66.4	26.91	22.9
	$4*A10 + 2*A12 + 2*A2 + 2*A9 + 2*A22*C22 + A69$ 1-methylnaphthalene					[221]
$C_{11}H_{10}$	4.98	20.69				
	6.95	28.62	49.3	44.9	11.92	10.9
$C_{11}H_{10}$	$A1 + 7*A10 + A11 + 2*A12$ 2-methylnaphthalene					[216]
	5.61	19.43				
$C_{11}H_{10}O_2$	12.13	39.43	58.87	44.9	17.74	13.8
	$A1 + 7*A10 + A11 + 2*A12$ 2-acetyl-1-naphthol					[216]
$C_{11}H_{10}O_2$	22.52	0	60.57	57.0	22.52	21.2
	$6*A10 + 4*A12 + A31 + A35 + A1$					[215]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$C_{11}H_{10}O_2$	1-acetyl-2-naphthol					
	21.34	0	63.32	57.0	21.34	19.2
$C_{11}H_{10}O_4$	$6*A10+4*A12+A31+A35+A1$					
	<i>p</i> -methacryloyloxybenzoic acid					
455	34	0	74.73	62.7	34	28.5
$C_{11}H_{11}Cl_3O_3$	$4*A10+2*A12+A36*B36+A38+A5+A7+A1$					
	methyl 2-(2,4,5-trichlorophenoxy)butyrate					
316.5	28.87	0	91.22	78.3	28.87	24.8
$C_{11}H_{12}NO_3PS$	$3*A22*E22+2*A1+4*A12+2*A10+A38+A32+A2+A3*B3$					
	O,O-dimethyl S-phthalimidomethyl phosphorodithioate					
343.2	26.96	0	78.56	79.7	26.96	27.3
$C_{11}H_{12}Cl_2O_3$	$A14+2*A15+A128+2*A19+4*A10+2*A1+A2+A80$					
	methyl 4-(2,4-dichlorophenoxy)butyrate					
309.6	32.64	0	105.41	83.5	32.64	25.9
$C_{11}H_{13}F_3N_2O_3S$	$2*A22*D22+A1+3*A12+3*A10+A38+A32+3*A2$					
	5'-(trifluoromethanesulphonamide)acet-2',4'-xylidide					
457.3	37.66	0	82.35	61.6	37.66	28.1
$C_{11}H_{13}ClO_3$	$3*A1+2*A10+2*A11+2*A12+A60+A4*B4+3*A25+A95$					
	4-(4-chloro-2-methylphenoxy)butanoic acid					
373.5	32.02	0	85.73	87.6	32.02	32.7
$C_{11}H_{13}NO_4$	$3*A10+2*A12+A11+A1+3*A2+A36*C36+A22*C22+A32$					
	2,3-diisopropylidenedioxyphenyl-N-methylcarbamate					
402.6	29.45	0	73.14	62.2	29.45	25.1
$C_{11}H_{13}F_3N_4O_4$	$A14+2*A15+2*A19+2*A112+A17+3*A1+A69+3*A10+A12$					
	N(3),N(3)-diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine					
372.1	29.13	0	78.29	69.1	29.13	25.7
$C_{11}H_{14}$	$4*A12+A10+A11+3*A25+A4*B4+2*A50+A45+A43+2*A1+2*A2$					
	pentacyclo[5.4.0.0[2,6].0[3,10].0[5,9]]undecane					
164.4	4.86	29.57				
475.8	6.38	13.41	42.98	34.3	11.24	16.3
$C_{11}H_{14}$	$5*A14-4*A15+8*A16$					
	1,1-dimethylindan					
227.4	11.99	0	52.73	46.5	11.99	10.6
$C_{11}H_{14}$	$A14+2*A15+A17+A1*2+2*A19+4*A10$					
	4,6-dimethylindan					
256.5	12.88	0	50.21	47.0	12.88	12.1
$C_{11}H_{14}$	$A14+2*A15+2*A19+2*A11+2*A10+2*A1$					
	4,7-dimethylindan					
272.7	13.52	0	49.58	47.0	13.52	12.8
$C_{11}H_{14}ClNO$	$A14+2*A15+2*A19+2*A11+2*A10+2*A1$					
	2-chloro-N-isopropyl N-phenylacetamide					
351.4	26.05	0	74.13	67.2	26.05	23.6
$C_{11}H_{14}O_2$	$5*A10+A12+2*A1+A3*B3+A2+A22*B22+A59$					
	4- <i>tert</i> -butylbenzoic acid					
440	17.91	0	40.7	43.8	17.91	19.3
$C_{11}H_{14}O_3$	$4*A10+A11+A12+A36+3*A1+A4$					
	(<i>dl</i>) 3-phenyl-3-hydroxy-2,2-dimethylpropanoic acid					
407	37.24	0	91.49	64.3	37.24	26.1
$C_{11}H_{14}O_3$	$5*A10+A11+A3*B3+A4*B4+2*A1+B30*A30+A36*B36$					
	(<i>d</i>) 3-phenyl-3-hydroxy-2,2-dimethylpropanoic acid					
431	39.75	0	92.22	64.3	39.45	27.7
$C_{11}H_{14}O_3$	$5*A10+A11+A3*B3+A4*B4+2*A1+B30*A30+A36*B36$					
	4-methoxyphenylbutyric acid					
330.9	25.3	0	76.46	72.4	25.3	24.0
$C_{11}H_{14}O_3$	$4*A10+A11+A12+3*A2+A1+A36*B36+A32$					
	(<i>dl</i>) 3-hydroxy-3-phenylvaleric acid					
394	35.15	0	89.2	70.7	35.15	27.9
$C_{11}H_{14}O_3$	$5*A10+A11+A1+2*A2+A4*B4+B36*A36+B30*A30$					
	(<i>d</i>) 3-hydroxy-3-phenylvaleric acid					
379	30.96	0	81.69	70.7	30.96	26.8
$C_{11}H_{15}N$	$5*A10+A11+A1+2*A2+A4*B4+A36*B36+B30*A30$					
	1-cyanoadamantane					
280	5.5	19.64				
458	15	32.75	52.39	42.8	20.5	19.6
$C_{11}H_{15}NO_2$	$3*A14+A15+3*A16+A17+A56$					
	4- <i>trans</i> -cyanocyclohexyl (E) 2-butenate					
						[148]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
366.2	24.4	0	66.63	67.2	24.4	24.6
$C_{11}H_{15}NO_2$	A14+3*A15+2*A16+A56+A38+A1+A6*B6+A6 butyl 4-aminobenzoate					[140]
331.1	20.46	0	61.79	82.7	20.46	27.4
$C_{11}H_{15}NO_2$	4*A10+2*A12+A1+A45+A38+3*A2 2-(1-methylethyl)phenyl methylcarbamate					[215]
369.3	26.14	0	70.78	59.6	26.14	22.0
$C_{11}H_{15}NO_2$	3*A1+A3+4*A10+A11+A12+A69 4-methylthio-3,5-xylol methylcarbamate					[221]
393.8	30.36	0	77.11	63.7	30.36	25.1
$C_{11}H_{15}NO_3$	4*A1+2*A11+2*A12+A69+A84+2*A10 1,2-dihydro-6-neopentyl-2-oxonicotinic acid					[215]
469.2	19.33	0	41.2	60.6	19.33	28.4
$C_{11}H_{15}N_3O_2$	A14+3*A15+A124+2*A18+2*A19+A36+3*A1+A2+A4 N-caproyl-pyrazinamide					[164]
351.7	35.95	0	102.22	90.4	35.95	31.8
$C_{11}H_{16}$	A1+4*A2+3*A10+A12+2*A41+A71 pentamethylbenzene					[9]
296.8	1.98	6.67				
328.2	10.67	32.51	39.33	47.3	12.65	15.5
$C_{11}H_{16}N_4O_2$	5*A1+A10+5*A11 8-butyltheophylline					[216]
509.2	32.3	0	63.43	74.5	32.3	37.9
$C_{11}H_{16}N_4O_2$	2*A14+3*A15+2*A125+A118+A121+3*A1+3*A19+3*A2 8-tert-butyltheophylline					[236]
402.3	48.2	0	119.81	53.4	48.2	21.5
$C_{11}H_{16}Si$	2*A14+3*A15+2*A125+A118+A121+2*A1+3*A19+3*A1+A4 vinyl dimethylbenzylsilane					[236]
204.1	11.6	0	56.83	65.3	11.6	13.3
$C_{11}H_{17}N_5$	2*A1+A2+A109+5*A10+A11+A5+A6 6,9-dimethyl-8-butyladenine					[216]
409.2	36	0	87.98	75.8	36	31.0
$C_{11}H_{18}$	A14+2*A15+3*A19+3*A1+A118+A119+2*A41+A10+A12+A44+3*A2 1-methyladamantane					[240]
169.5	1.91	11.27				
211.5	1.47	6.95				
392	3.71	9.46	27.68	42.7	7.09	16.7
$C_{11}H_{19}NO_3$	3*A14+A15+3*A16+A17+A1 2-isopropoxyphenyl N-methylcarbamate					[146]
363.1	22.96	0	63.23	72.9	22.96	26.5
$C_{11}H_{19}NS$	3*A1+A69+A3*B3+4*A10+2*A12+A32 2,4-di-tert-butylthiazole					[215]
258.2	10.5	0	40.67	52.4	10.5	13.5
$C_{11}H_{19}N_3O$	A14+2*A15+2*A19+A18*B18+6*A1+2*A4+A131+A118 5-butyl-2-ethylamino-6-methylpyrimidin-4-ol					[61]
432.5	20.32	0	46.98	83.9	20.32	36.3
$C_{11}H_{19}N_5S$	2*A11+2*A12+3*A1+3*A2+A44+A31+2*A41+A2 6-ethylthio-N,N'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine					[215]
377.7	23.94	0	63.38	77.2	23.94	29.2
$C_{11}H_{20}N_6$	3*A41+3*A12+5*A1+2*A3*B3+A2+A84+2*A44 1-pyrrolidinyl-3,5-bis(dimethylamino)-s-triazine					[215]
403.1	25.61	0	63.53	57.6	25.61	23.2
$C_{11}H_{20}N_6O$	A14+2*A15+A119+4*A1+2*A43+3*A12+3*A41 1-morpholinyl-3,5-bis(dimethylamino)-s-triazine					[215]
397.4	24.69	0	62.13	62.5	24.69	24.8
$C_{11}H_{20}N_7S$	A14+3*A15+A119+A112+4*A1+2*A43+3*A41+3*A12 1-(thiomorpholinyl)-3,5-bis(dimethylamino)-s-triazine					[215]
391.2	29.08	0	74.33	64.2	29.08	25.1
$C_{11}H_{20}O_2$	4*A1+2*A43+3*A41+3*A12+A14+3*A15+A119+A131 undecanolactone					[215]
250.2	3.36	13.43				
275.3	12.61	45.8	59.23	69.8	15.97	19.2
$C_{11}H_{20}O_4$	A14+9*A15+A115 undecanedioic acid					[216]
385	39.65	0	102.99	116.2	39.65	44.7
$C_{11}H_{21}N_5S$	9*A2*B2+2*A36*B36 6-(ethylthio)-N,N'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
377.7	23.94	0	63.39	77.2	23.94	29.2
$C_{11}H_{21}N_7$	$5*A1 + A2 + 2*A3*B3 + 3*A41 + 2*A44 + A84 + 3*A12$ 1-(piperiziny)-3,5-bis(dimethylamino)-s-triazine					[221]
382	23.01	0	60.24	63.5	23.01	24.3
$C_{11}H_{22}$	$4*A1 + 2*A43 + 3*A41 + 3*A12 + A14 + 3*A15 + A119 + A121$ 1-undecene					[215]
217.3	9.2	42.36				
224	16.99	75.84	118.2	114.8	26.19	25.7
$C_{11}H_{22}O$	$A1 + 8*A2*B2 + A5 + A6$ 2-undecanone					[216]
290.5	28.78	0	99.07	114.4	28.78	33.2
$C_{11}H_{22}O_2$	$2*A1 + 8*A2*B2 + A35$ undecanoic acid					[21]
290	8.13	28.03				
301.6	25.98	86.15	114.22	114.9	34.11	34.7
$C_{11}H_{24}$	$9*A2*B2 + A1 + A36$ <i>n</i> -undecane					[216]
236.6	6.86	29				
247.6	22.18	89.6	118.6	119.1	29.03	29.5
$C_{11}H_{24}$	$2*A1 + 9*A2*B2$ 2-methyldecane					[216]
224.3	25.06	0	111.73	101.7	25.06	22.8
$C_{11}H_{24}O$	$3*A1 + 7*A2*B2 + A3$ methyl <i>n</i> -decyl ether					[216]
243.5	31.71	0	130.12	123.8	31.71	30.2
$C_{11}H_{24}O_2S$	$2*A1 + 9*A2*B2 + A32$ 3(<i>n</i> -octylthio)-1,2-propanediol					[216]
306.5	39.8	0	129.85	123.4	39.8	37.8
$C_{11}H_{24}O_3$	$A1 + 7*A2*B2 + A84 + 2*A30*C30 + A3*B3 + 2*A2$ 3(<i>n</i> -octyloxy)-1,2-propanediol					[217]
296.1	33.4	0	112.8	126.0	33.4	37.3
$C_{11}H_{25}NO_2$	$A1 + 7*A2*B2 + A32 + 2*A30*C30 + A3*B3 + 2*A2$ 3(<i>n</i> -octylamino)-1,2-propanediol					[217]
335.9	45.1	0	134.27	116.0	45.1	39.0
$C_{12}Cl_{10}$	$A1 + 7*A2*B2 + A44 + 2*A30*C30 + A3*B3 + 2*A2$ decachlorobiphenyl					[217]
577.7	39.34	0	68.1	72.1	39.34	41.6
$C_{12}F_{26}$	$12*A12 + 10*A22*G22$ perfluorododecane					[215]
170.2	6.9	40.54				
348.5	38.16	109.5	150.0	133.3	45.06	46.4
$C_{12}HCl_9$	$12*A4*B4 + 6*A25 + 20*A26$ 2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl					[67]
455.8	22.6	0	49.58	70.8	22.6	32.3
$C_{12}H_2Cl_8$	$11*A12 + 9*A22*G22 + A10$ 2,2',3,3',5,5',6,6'-octachlorobiphenyl					[215]
433.8	22.8	0	52.56	69.5	22.8	30.1
$C_{12}H_3Cl_7$	$10*A12 + 8*A22*G22 + 2*A10$ 2,2',3,3',5,5',6-heptachlorobiphenyl					[215]
395.4	20.3	0	51.34	68.2	20.3	27.0
$C_{12}H_4Cl_6$	$9*A12 + 7*A22*G22 + 3*A10$ 2,2',3,3',5,5'-hexachlorobiphenyl					[215]
424.9	29.2	0	68.72	66.9	29.2	28.4
$C_{12}H_4Cl_6$	$6*A22*F22 + 4*A10 + 8*A12$ 2,2',3,3',6,6'-hexachlorobiphenyl					[215]
385.2	21.1	0	54.78	66.9	21.1	25.8
$C_{12}H_4Cl_6$	$6*A22*F22 + 4*A10 + 8*A12$ 2,2',4,4',6,6'-hexachlorobiphenyl					[215]
386.7	17.5	0	45.25	66.9	17.5	25.9
$C_{12}H_5Cl_5O_2$	$6*A22*F22 + 4*A10 + 8*A12$ 1,3,7-trichlorodibenzodioxin					[215]
421.7	30.8	0	73.04	61.0	30.8	25.7
$C_{12}H_5Cl_5$	$A14 + 3*A15 + 2*A112 + 3*A22*E22 + 4*A19 + 5*A10 + 3*A12$ 2,2',4,5,5'-pentachlorobiphenyl					[20]
350.1	18.8	0	53.7	65.6	18.8	23.0
$C_{12}H_5Cl_5$	$5*A22*E22 + 5*A10 + 7*A12$ 2,3,4,5,6-pentachlorobiphenyl					[215]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
397.6	21.8	0	54.83	65.6	21.8	26.1
$\text{C}_{12}\text{H}_6\text{Cl}_2\text{O}$	$5^*A22^*E22+5^*A10+7^*A12$ 3,6-dichlorodibenzofuran					[215]
461.2	32.4	0	70.25	54.8	32.4	25.3
$\text{C}_{12}\text{H}_6\text{Cl}_4$	$A14+2^*A15+2^*A19+2^*A19+A112+2^*A22^*C22+6^*A10+2^*A12$ 2,2',4',5-tetrachlorobiphenyl					[20]
339.1	23.4	0	69.01	64.3	23.4	21.8
$\text{C}_{12}\text{H}_6\text{Cl}_4$	$6^*A12+6^*A10+4^*A22^*D22$ 2,3,4,5-tetrachlorobiphenyl					[215]
363.9	25.2	0	69.25	64.3	25.2	23.4
$\text{C}_{12}\text{H}_6\text{Cl}_4\text{O}_2\text{S}$	$6^*A12+6^*A10+4^*A22^*D22$ 1,2,4-trichloro-5-((4-chlorophenyl)sulfonyl)benzene					[215]
419.9	28.94	71.21	68.92	64.6	28.94	27.1
$\text{C}_{12}\text{H}_6\text{O}_3$	$6^*A12+6^*A10+4^*A22^*E22+A88$ 1-8-naphthalic anhydride					[215]
542.3	23.32	0	43	47.0	23.32	22.5
$\text{C}_{12}\text{H}_6\text{S}$	$A14+3^*A15+3^*A19+A117+6^*A10+A12$ dibenzothiophene					[221]
373.2	21.6	0	57.74	53.9	21.6	20.1
$\text{C}_{12}\text{H}_7\text{ClO}_2$	$8^*A10+A131+A14+2^*A15+4^*A19$ 1-chlorodibenzodioxin					[283]
378.2	23.2	0	61.34	58.5	23.2	22.1
$\text{C}_{12}\text{H}_7\text{ClO}_2$	$A14+3^*A15+2^*A112+4^*A19+A12+7^*A10+A22^*C22$ 2-chlorodibenzodioxin					[20]
362.2	23.1	0	63.78	58.5	23.1	21.2
$\text{C}_{12}\text{H}_7\text{Cl}_2\text{NO}_3$	$A14+3^*A15+2^*A112+4^*A19+A12+7^*A10+A22^*C22$ 2,4-dichlorophenyl 4-nitrophenyl ether					[20]
342	22.96	0	67.13	69.3	22.96	23.7
$\text{C}_{12}\text{H}_7\text{Cl}_3$	$7^*A10+5^*A12+2^*A22^*D22+A50+A32$ 2,4,6-trichlorobiphenyl					[221]
334.3	16.5	0	49.36	63.0	16.5	21.1
$\text{C}_{12}\text{H}_7\text{Cl}_3$	$5^*A12+7^*A10+3^*A22^*C22$ 2,4,5-trichlorobiphenyl					[215]
349.5	22.8	0	65.24	63.0	22.8	22.0
C_{12}H_8	$5^*A12+7^*A10+3^*A22^*C22$ acenaphthylene					[215]
116.6	1.4	12.12				
362.6	6.95	19.15	31.27	37.8	8.36	13.7
362.0	10.96	30.28	42.40	37.8	12.36	13.7
$\text{C}_{12}\text{H}_8\text{Br}_2$	$A14+2^*A15+3^*A19+6^*A10+A12+2^*A16$ (dl) 1,2-dibromoacenaphthene					[216,154]
397	25.1	0	63.22	46.4	25.1	18.4
$\text{C}_{12}\text{H}_8\text{Br}_2$	$6^*A10+A14+2^*A15+2^*A21+2^*A16+A12+3^*A19$ (d) 1,2-dibromoacenaphthene					[273]
416	26.36	0	63.35	46.4	26.36	19.3
$\text{C}_{12}\text{H}_8\text{Cl}_2$	$6^*A10+A14+2^*A15+2^*A21+2^*A16+A12+3^*A19$ (dl) 1,2-dichloroacenaphthene					[273]
339	20.5	0	60.46	43.9	20.5	14.9
$\text{C}_{12}\text{H}_8\text{Cl}_2$	$2^*A15+A14+6^*A10+2^*A22^*B22+2^*A16+3^*A19$ (d) 1,2-dichloroacenaphthene					[273]
375	21.34	0	56.9	43.9	21.34	16.5
$\text{C}_{12}\text{H}_8\text{Cl}_2$	$2^*A15+A14+6^*A10+2^*A22^*B22+2^*A16+3^*A19$ 2,6-dichlorobiphenyl					[273]
307.9	12.6	0	40.92	61.8	12.6	19.0
$\text{C}_{12}\text{H}_8\text{Cl}_2\text{O}_2\text{S}$	$4^*A12+8^*A10+2^*A22^*B22$ 4,4'-dichlorodiphenylsulphone					[215]
422	24.4	0	57.82	62.0	24.4	26.2
$\text{C}_{12}\text{H}_8\text{Cl}_2\text{O}_3\text{S}$	$8^*A10+4^*A12+2^*A22^*C22+A88$ 4-chlorophenyl 4-chlorobenzenesulfonate					[216]
360.0	23.63	0	65.64	69.7	23.63	25.1
$\text{C}_{12}\text{H}_8\text{Cl}_6\text{O}$	$8^*A10+4^*A12+2^*A22^*C22+A89$ 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4 α ,5,6,7,8,8 α -octahydro-1,4-endo, exo-5,8-dimethanonaphthalene (Dieldrin)					[215]
405.6	19.33	47.66				
452.9	3.04	6.71	54.37	41.2	22.37	18.7
$\text{C}_{12}\text{H}_8\text{Cl}_6\text{O}$	$5^*A14-2^*A15+6^*A22^*G22+3^*A17+2^*A19+4^*A16+2^*A16+A112$ 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4 α ,5,6,7,8,8 α -octahydro-1,4-endo,					[222]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
	endo-5,8-dimethanonaphthalene (Endrin)					
383.7	16.59	43.24				
562.4	4.15	7.38	50.62	41.2	20.74	23.2
$\text{C}_{12}\text{H}_8\text{N}_2$	5*A14-2*A15+6*A22*G22+3*A17+2*A19+6*A16+A112					
	phenazine					
450.2	20.92	0	46.47	51.2	20.92	23.1
$\text{C}_{12}\text{H}_8\text{N}_2$	8*A10+4*A12+2*A41					
	benzo[c]cinnoline					
432.2	20.92	0	48.4	51.2	20.92	22.1
$\text{C}_{12}\text{H}_8\text{N}_2\text{O}_5$	8*A10+4*A12+2*A41					
	4,4'-dinitrodiphenyl ether					
418.2	10.29	0	24.61	69.6	10.29	29.1
$\text{C}_{12}\text{H}_8\text{O}$	8*A10+4*A12+2*A50+A32					
	dibenzofuran					
355.7	18.6	0	52.29	52.3	18.6	18.6
$\text{C}_{12}\text{H}_8\text{OS}$	A14+2*A15+A112+2*A19+8*A10+2*A19					
	phenoxathiin					
328.8	20.27	0	61.63	58.9	20.27	19.4
$\text{C}_{12}\text{H}_8\text{OS}_2$	3*A15+A14+4*A19+8*A10+A131+A112					
	diphenylene-2,2'-disulfide S-oxide					
407	17.99	0	44.2	56.6	17.99	23.1
$\text{C}_{12}\text{H}_8\text{O}_2$	8*A10+A14+3*A15+4*A19+A133					
	dibenzodioxin					
395.7	23.2	0	58.63	57.2	23.2	22.6
$\text{C}_{12}\text{H}_8\text{S}$	A14+3*A15+4*A19+8*A10+2*A112					
	dibenzothiophene					
371	21.58	0	58.17	53.9	21.58	20.0
$\text{C}_{12}\text{H}_8\text{S}_2$	A14+2*A15+2*A19+2*A19+A131+8*A10					
	dibenzo[c,e][1,2]dithiin					
386.2	19.3	0	49.97	48.3	19.3	18.7
$\text{C}_{12}\text{H}_8\text{S}_2$	A14+3*A15+2*A19+2*A19+8*A10+A132					
	thianthrene					
429.6	27.55	0	64.13	60.5	27.55	26.0
$\text{C}_{12}\text{H}_9\text{Cl}$	3*A15+A14+8*A10+4*A19+2*A131					
	2-chlorobiphenyl					
304.9	14.54	0	47.7	55.1	14.54	16.8
$\text{C}_{12}\text{H}_9\text{Cl}$	3*A12+9*A10+A22					
	4-chlorobiphenyl					
348.6	13.32	0	38.2	55.1	13.32	19.2
$\text{C}_{12}\text{H}_9\text{ClN}_2$	2*A12+9*A10+A22+A12					
	4-chloroazobenzene					
361.2	27.2	0	75.3	57.0	27.2	20.6
$\text{C}_{12}\text{H}_8\text{Cl}_2\text{O}_3\text{S}$	9*A10+3*A12+2*A42+A22*B22					
	4-chlorophenylbenzenesulfonate					
332.2	21.44	0	64.53	68.4	21.44	22.7
$\text{C}_{12}\text{H}_9\text{Cl}_3\text{Si}$	9*A10+3*A12+A22*B22+A89					
	o-trichlorosilylbiphenyl					
289.5	0.06	0.2				
339.2	20.72	61.09	61.28	63.6	20.78	21.6
$\text{C}_{12}\text{H}_9\text{Cl}_3\text{Si}$	9*A10+2*A12+A11+3*A22*D22+A109					
	p-trichlorosilylbiphenyl					
372.9	18.57	0	49.8	63.6	18.57	23.7
$\text{C}_{12}\text{H}_9\text{Cl}_3\text{Si}$	9*A10+2*A12+A11+3*A22*D22+A109					
	4-trichlorosilylbiphenyl					
372.9	18.57	0	49.8	65.8	18.57	24.5
$\text{C}_{12}\text{H}_9\text{N}$	9*A10+3*A12+A109+3*A22*D22					
	carbazole					
521	27.2	0	52.2	53.2	27.2	27.5
$\text{C}_{12}\text{H}_9\text{NS}$	A14+2*A15+2*A19+2*A19+8*A10+A121					
	10H-phenothiazine					
458.2	26.92	0	58.75	59.8	26.92	27.4
$\text{C}_{12}\text{H}_{10}$	A14+3*A15+4*A19+8*A10+A121+A131					
	acenaphthene					
366.6	21.46	0	58.55	41.09	21.46	15.0
$\text{C}_{12}\text{H}_{10}$	6*A10+A14+2*A15+3*A19+A12					
	biphenyl					
341.5	18.66	0	54.81	59.2	18.66	20.2

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_{12}\text{H}_{10}\text{N}_2$	10*A10+2*A12 <i>trans</i> -azobenzene 22.53	0	66.06	55.7	22.53	19.0 [216]
$\text{C}_{12}\text{H}_{10}\text{N}_2\text{O}$	10*A10+2*A12+2*A42 azoxybenzene 17.93	0	57.99	64.3	17.93	19.9 [215]
$\text{C}_{12}\text{H}_{10}\text{N}_2\text{O}$	10*A10+2*A12+A54+A42 4-hydroxyazobenzene 32.99	0	77.59	61.0	32.99	26.0 [13]
$\text{C}_{12}\text{H}_{10}\text{N}_4\text{O}_2$	9*A10+3*A12+2*A42+A31 4-(4-nitrophenylazo)aniline 31.88	0	65.3	65.0	31.88	31.7 [13]
$\text{C}_{12}\text{H}_{10}\text{O}$	8*A10+4*A12+2*A42+A50+A45 <i>o</i> -hydroxybiphenyl 16.21	0	48.12	64.6	16.21	21.3 [63]
$\text{C}_{12}\text{H}_{10}\text{O}$	9*A10+A31+3*A12 diphenyl ether 17.21	0	57.32	63.9	17.21	19.2 [216]
$\text{C}_{12}\text{H}_{10}\text{O}_2$	10*A10+2*A12+A32 1-naphthaleneacetic acid 22.26	0	54.92	47.8	22.26	19.4 [215]
$\text{C}_{12}\text{H}_{10}\text{O}_2$	7*A10+2*A12+A11+A2+A36 2-carbomethoxynaphthalene 27.1	0	77.4	54.7	27.1	19.2 [247]
$\text{C}_{12}\text{H}_{10}\text{O}_2$	7*A10+A1+A38+3*A12 1-acetoxynaphthalene 20.21	0	63.31	54.7	20.21	17.5 [118]
$\text{C}_{12}\text{H}_{10}\text{O}_2$	7*A10+3*A12+A1+A38 2-acetoxynaphthalene 20.05	0	58.59	54.7	20.05	18.7 [118]
$\text{C}_{12}\text{H}_{11}\text{Cl}_2\text{NO}$	7*A10+3*A12+A1+A38 3,5-dichloro-N-(1,1-dimethyl-2-propynyl)benzamide 28.68	0	66.94	58.1	28.68	24.9 [221]
$\text{C}_{12}\text{H}_{11}\text{N}$	3*A12+3*A10+A60+2*A22*C22+2*A1+A4*B4+A8+A9 diphenylamine 17.86	0	54.75	53.9	17.86	17.6 [215]
$\text{C}_{12}\text{H}_{11}\text{N}$	10*A10+2*A12+A44 2-aminobiphenyl 13.99	0	43.4	65.7	13.99	21.2 [205]
$\text{C}_{12}\text{H}_{11}\text{NO}$	9*A10+3*A12+A45 1-naphthaleneacetamide 32.82	0	72.05	62.4	32.82	28.4 [221]
$\text{C}_{12}\text{H}_{11}\text{NO}_2$	7*A10+2*A12+A11+A2+A61 1-naphthyl methylcarbamate 24.51	0	58.88	57.6	24.51	24.0 [221]
$\text{C}_{12}\text{H}_{11}\text{N}_3$	7*A10+3*A12+A1+A69 <i>p</i> -phenylazoaniline 21.7	0	54.5	62.1	21.7	24.7 [13]
$\text{C}_{12}\text{H}_{12}$	9*A10+3*A12+2*A42+A45 1,8-dimethylnaphthalene 15.77	0	46.9	45.5	15.77	15.3 [215]
$\text{C}_{12}\text{H}_{12}$	2*A1+2*A11+6*A10+2*A12 2,6-dimethylnaphthalene 25.06	0	65.39	45.5	25.06	17.4 [215]
$\text{C}_{12}\text{H}_{12}$	2*A1+2*A11+6*A10+2*A12 2,7-dimethylnaphthalene 23.35	0	63.3	45.5	23.35	16.8 [215]
$\text{C}_{12}\text{H}_{12}$	2*A1+2*A11+6*A10+2*A12 1,4-dimethylnaphthalene 10.6	0	37.87	45.5	10.6	12.7 [215]
$\text{C}_{12}\text{H}_{12}$	2*A1+2*A11+2*A12+6*A10 2,3-dimethylnaphthalene 15.9	0	42.06	45.5	15.9	17.2 [215]
$\text{C}_{12}\text{H}_{12}\text{Ge}$	2*A1+2*A11+2*A12+6*A10 diphenylgermane 11.91	0	49.58	44.5	11.91	10.7

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}S_{\text{tpce}}}$ (expt)	$\Delta_0^{T_{\text{fus}}S_{\text{tpce}}}$ (calcd)	$\Delta_0^{T_{\text{fus}}H_{\text{tpce}}}$ (expt)	$\Delta_0^{T_{\text{fus}}H_{\text{tpce}}}$ (calcd)
$\text{C}_{12}\text{H}_{12}\text{N}_2$	10*A10+2*A12+A103 hydrazobenzene					[133]
407.2	17.65	0	43.34	48.6	17.65	19.8
$\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}$	10*A10+2*A12+2*A44 4'4'-diaminodiphenyl ether					[215]
465.4	7.74	0	16.63	76.8	7.74	35.8
$\text{C}_{12}\text{H}_{12}\text{O}_4$	8*A10+4*A12+2*A45+A32 1,4-dimethylcubane dicarboxylate					[216]
437.8	41	0	93.65	34.0	41	14.9
$\text{C}_{12}\text{H}_{12}\text{O}_6$	5*A14-7*A15+6*A16+2*A17+2*A1+2*A38 1,2,3-tricarboxymethoxybenzene					[340]
375.7	32.7	0	87.04	75.6	32.7	28.4
$\text{C}_{12}\text{H}_{13}\text{ClF}_3\text{N}_3\text{O}_4$	3*A1+3*A38+3*A12+3*A10 N-(2-chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzeneamine					[217]
318.4	23.08	0	72.49	75.5	23.08	24.0
$\text{C}_{12}\text{H}_{13}\text{NO}_2$	2*A10+3*A112+A11+4*A2+A1+A4*B4+3*A25+2*A50+A43+A22*G22 4-methyl-7-dimethylaminocoumarin					[221]
416.1	23.92	0	57.47	53.0	23.92	22.0
$\text{C}_{12}\text{H}_{13}\text{NO}_4\text{S}$	A14+3*A15+A115+2*A19+A19+A18*B18+3*A1+3*A10+A12+A43 2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathiin-4,4-dioxide					[216]
401.5	26.66	0	66.39	59.4	26.66	23.8
$\text{C}_{12}\text{H}_{14}\text{N}_2\text{O}_5$	A14+3*A15+A112+A1+2*A19+A134+A60+5*A10+A12 2-cyclohexyl-4,6-dinitrophenol					[221]
378.7	28.03	0	74.02	68.3	28.03	25.9
$\text{C}_{12}\text{H}_{14}\text{N}_4\text{O}$	A14+3*A15+A16+2*A10+A11+3*A12+A31+2*A50 3,3',4,4'-tetraaminodiphenyl ether					[232]
402.6	25.3	0	62.84	89.8	25.3	36.2
$\text{C}_{12}\text{H}_{14}\text{O}_4$	4*A45+6*A12+6*A10+A32 diethyl <i>o</i> -phthalate					[227]
269.9	17.99	0	66.66	79.5	17.99	21.5
$\text{C}_{12}\text{H}_{14}\text{O}_4$	4*A10+2*A38+2*A12+2*A2+2*A1 diethyl terephthalate					[216]
317.2	24.69	0	77.82	79.5	24.69	25.2
$\text{C}_{12}\text{H}_{15}\text{ClNO}_4\text{S}_2$	4*A10+2*A38+2*A12+2*A2+2*A1 S-6-chloro-2,3-dihydro-2-oxobenzoxazol-3-ylmethyl O,O-diethyl phosphorodithioate					[216]
320.0	30.03	0	93.86	89.0	30.03	28.5
$\text{C}_{12}\text{H}_{15}\text{NO}_2$	A14+2*A15+A126+2*A19+3*A10+A12+A22*C22+3*A2+2*A1+A80 phenylaminoethyl methacrylate					[221]
297.5	25.47	0	85.6	70.4	25.47	21.0
$\text{C}_{12}\text{H}_{15}\text{NO}_3$	5*A10+A12+A44+2*A2+A1+A5+A7+A38 2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate					[216]
426.24	30.33	0	71.17	61.0	30.33	26.0
$\text{C}_{12}\text{H}_{15}\text{N}_2\text{O}_3\text{PS}$	A14+2*A15+A17+2*A19+A112+3*A10+A12+3*A1+A69 O,O-diethyl O-quinoxalin-2-yl phosphothioate					[221]
304.1	25.4	0	83.5	87.0	25.4	26.5
$\text{C}_{12}\text{H}_{15}\text{N}_5\text{O}_4$	5*A10+3*A12+2*A41+2*A1+2*A2+A79 9-[(2-acetoxyethoxy)methyl]-2-acetylamino-9H-purine					[221]
407.2	42.33	0	104.0	86.5	42.33	35.2
$\text{C}_{12}\text{H}_{15}\text{N}_5\text{O}_5$	A14+2*A15+2*A19+A18*B18+A118+A119+ 2*A41+A10+A12+A60+2*A1+3*A2+A38+A32 9-[(2-acetoxyethoxy)methyl]-2-acetylamino-1,9-dihydro-6H-purin-6-one					[203]
477.2	47.37	0	99.27	92.8	47.37	44.3
$\text{C}_{12}\text{H}_{16}$	2*A14+3*A15+3*A19+A18*B18+2*A118+A119+A124+A60+2*A1+3*A2+A38+A32 cyclohexylbenzene					[203]
280.5	15.3	0	54.55	57.2	15.3	16.1
$\text{C}_{12}\text{H}_{16}\text{Cl}_2\text{N}_2\text{O}$	A14+3*A15+5*A10+A11+A16 N-butyl-N'-(3,4-dichlorophenyl)-N-methylurea					[216]
374.3	27.23	0	72.75	86.2	27.23	32.3
$\text{C}_{12}\text{H}_{16}\text{NO}_2$	2*A1+3*A2+3*A10+3*A12+2*A22*C22+A64*B64 5-isopropyl- <i>m</i> -tolyl methylcarbamate					[221]
361.3	23.04	0	63.77	60.1	23.04	21.7
$\text{C}_{12}\text{H}_{16}\text{N}_2\text{O}_2$	4*A1+A3+2*A11+A12+3*A10+A69 4-dimethylamino-3,5-xylyl methylcarbamate					[221]
361.7	18.37	0	50.78	56.9	18.37	20.6
	5*A1+2*A10+2*A11+2*A12+A69+A43					[221]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)	
$C_{12}H_{16}N_3O_6S$	424.3	4-methylsulphonyl-2,6-dinitro-N,N-dipropylaniline 28.05	0	66.1	79.7	28.05	33.8
$C_{12}H_{16}N_3O_3PS_2$	322.2	$3*A1 + 4*A2 + 4*A12 + 2*A10 + A43 + 2*A50 + A88$ S-(3,4-dihydro-4-oxobenzo[d]-[1,2,3]-triazin-3-ylmethyl) O,O-diethyl phosphorodithioate 25.22	0	78.26	75.9	25.22	24.4
$C_{12}H_{17}NO_2$	325.1	$A14 + 3*A15 + 2*A118 + 2*A19 + 4*A10 + A125 + 3*A2 + 2*A1 + A80$ pentyl 4-aminobenzoate 23.93	0	73.61	89.9	23.93	29.2
$C_{12}H_{18}$	383.7 438.7	$4*A10 + 2*A12 + A1 + 4*A2 + A45 + A38$ hexamethylbenzene 1.76	4.58				
$C_{12}H_{18}N_2O$	430.5	$6*A1 + 6*A11$ N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]urea 33.87	0	78.68	66.7	33.87	28.7
$C_{12}H_{18}N_2O_2$	361.7	$4*A1 + A3 + 4*A10 + A11 + A12 + A64$ 3,5-dimethyl-4-(dimethylamino)phenyl methylcarbamate 18.37	0	50.79	56.9	18.37	20.6
$C_{12}H_{18}N_4O_2$	498.4	$5*A1 + 2*A10 + 2*A11 + 2*A12 + A43 + A69$ 8-pentyltheophylline 35.1	0	70.43	81.6	35.1	40.7
$C_{12}H_{18}N_4O_6S$	414.8	$2*A14 + 3*A15 + 2*A125 + A118 + A121 + 3*A1 + 3*A19 + 4*A2$ 4-(N,N-dipropylamino)-3,5-dinitrobenzenesulphonamide 38.48	0	92.78	90.2	38.48	37.4
$C_{12}H_{18}O_2$	341.5	$2*A1 + 4*A2 + 2*A10 + 4*A12 + 2*A50 + A43 + A96$ 4-hexylresorcinol 19.04	0	55.75	91.5	19.04	31.2
$C_{12}H_{19}ClNO_3$	332.0	$3*A10 + A11 + 2*A12 + A1 + 5*A2 + 2*A31$ N-methyl O-methyl O-2-chloro-4- <i>tert</i> -butylphenyl phosphoramidate 21.98	0	66.19	66.2	21.98	22.0
$C_{12}H_{20}$	221 245	$5*A1 + A4 + 2*A12 + A11 + 3*A10 + A78 + A22*B22$ 1,3-dimethyladamantane 7.36	33.3				
$C_{12}H_{20}N_4O_2$	389.6	0.92 $3*A14 + A15 + 2*A16 + 2*A17 + 2*A1$ 3-cyclohexyl-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione 20.36	3.76	37.06	40.4	8.28	9.9
$C_{12}H_{20}O_2$	405.2	$2*A14 + 6*A15 + 2*A125 + A16 + 3*A1 + 3*A43 + A19 + A118$ 1,7-cyclododecanedione 15.77	0	38.93	64.0	15.77	25.9
$C_{12}H_{20}O_3$	344.2	$A14 + 9*A15 + 2*A114$ 3,3,6,6-tetramethyloctanedioic anhydride 18.83	0	54.7	59.1	18.83	20.33
$C_{12}H_{20}O_4$	296.2	$A14 + 6*A15 + 4*A1 + 2*A17 + A117$ 1,5-cyclooctanedione bis ethylene ketal 18.03	0	60.88	61.8	18.03	18.3
$C_{12}H_{22}$	256.1 267.5 273.5 277.2	$3*A14 + 7*A15 + 4*A112 + 2*A17$ bicyclohexyl 1.54	6.01				
$C_{12}H_{22}N_2O_2$	517.4 617.8	$2*A14 + 6*A15 + 2*A16$ 1,8-diaza-2,9-dioxocyclotetradecane 13.6	26.29				
$C_{12}H_{22}N_6$	361.5	49.3 $A14 + 11*A15 + 2*A124$ 1-(piperidinyl)-3,5-(dimethylamino)-s-triazine 23.22	79.8	106.1	79.5	62.9	49.1
$C_{12}H_{22}O_2$	230.3	$A14 + 3*A15 + A119 + 4*A1 + 2*A43 + 3*A12 + 3*A41$ octyl methacrylate 24.9	0	104.6	114.8	24.9	26.4
$C_{12}H_{22}O_2$	236.5	$2*A1 + A7 + A5 + A38 + 7*A2*B2$ nonyl acrylate 23.36	0	98.78	121.2	23.36	28.7
		$A1 + A6*B6 + A5 + A38 + 8*A2*B2$					28.7

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
$C_{12}H_{22}O_4$	402.5	dodecanedioic acid 50.57	0	125.64	50.6	50.53 [216]
$C_{12}H_{22}O_4$	244.1	10*A2*B2 + 2*A36*B36 di- <i>n</i> -butyl succinate 29.21	0	119.65	29.21	26.3 [216]
$C_{12}H_{23}N_7$	354.2	2*A1 + 8*A2 + 2*A38 1-(4'-methylpiperiziny)-3,5-bis(dimethylamino)- <i>s</i> -triazine 20.42	0	57.65	20.42	21.1 [242]
$C_{12}H_{24}$	199 333.8	5*A1 + 2*A43 + 3*A41 + 3*A12 + A14 + 3*A15 + 2*A119 cyclododecane 0.6	3.02	47.35	15.4	22.3 [181]
$C_{12}H_{24}$	212.9 237.9	A14 + 9*A15 1-dodecene 4.55	21.38	104.92	24.43	29.5 [216]
$C_{12}H_{24}N_2O_2$	452	19.87 A1 + 9*A2*B2 + A5 + A6 N,N'-di- <i>n</i> -propyladipamide 36.11	0	79.91	36.11	43.0 [282]
$C_{12}H_{24}O_2$	316.9	4*A2 + 2*A1 + 2*A60 + 4*A2 dodecanoic acid 36.65	0	115.7	36.7	39.4 [216]
$C_{12}H_{24}O_4$	383.0	10*A2*B2 + A1 + A36 2,2,8,8-tetramethyl-1,3,7,9-tetraoxacyclododecane 23.4	0	61.1	23.4	27.9 [47]
$C_{12}H_{24}O_4$	332.0	A14 + 9*A15 + 4*A112 + 4*A1 + 2*A17 1,3,9,11-tetraoxacyclohexadecane 35.56	0	107.1	35.56	28.7 [117]
$C_{12}H_{24}O_6$	312.2	A14 + 13*A15 + 4*A112 1,4,7,10,13,16-hexaoxacyclooctadecane 34	0	108.9	34	30.0 [120]
$C_{12}H_{25}NO_3$	387.6	A14 + 15*A15 + 6*A112 N-decylglycine 42.2	0	108.9	42.2	46.3 [249]
$C_{26}H_{26}$	263.6	A19 + 9*A2*B2 + A44 + A36*B36 + A2 dodecane 36.82	0	139.75	36.82	33.9 [216]
$C_{12}H_{26}O$	300.2	2*A1 + 10*A2*B2 1-dodecanol 40.17	0	133.76	40.17	36.6 [217]
$C_{12}H_{26}O_3$	297.2	11*A2*B2 + A1 + A30 3-(<i>n</i> -nonyloxy)-1,2-propanediol 29.5	0	99.26	29.5	40.3 [217]
$C_{12}H_{27}ClSn$	260.2	A1 + 8*A2*B2 + A32 + 2*A30*C30 + A3*B3 + 2*A2 tri- <i>n</i> -butyltin chloride 11.43	0	43.93	11.43	28.3 [130]
$C_{12}H_{30}O_3Si_3$	160 242.3 280.2	3*A1 + 9*A2 + A22*B22 + A110 1,1,3,3,5,5-hexaethylcyclotrisiloxane 0.46	2.89	92.46	23.71	25.9 [227]
$C_{12}H_{36}Si_6$	352.4 528.8	6*A1 + 6*A2 + 3*A112 + 3*A139 + A14 + 3*A15 cyclododecamethylhexasilane 16.7	47.39	55.33	20.9	25.0 [175]
$C_{13}H_5N_3O_7$	430.2 449.2	A14 + 3*A15 + 6*A139 + 12*A1 2,4,7-trinitrofluoren-9-one 2.9	6.74	59.06	26.4	22.8 [198]
$C_{13}H_6Cl_6O_2$	437.6	23.5 A14 + 2*A15 + 2*A19 + 2*A19 + 4*A10 + 3*A12 + 3*A50 + A114 2,2'-methylenebis(3,4,6-trichlorophenol) 33.26	0	76.01	33.26	35.3 [215]
$C_{13}H_7F_3N_2O_5$	364.6	2*A10 + 8*A12 + 2*A11 + 6*A22*G22 + A2 + 2*A31 2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene 18.44	0	50.58	18.44	25.3 [215]
$C_{13}H_8Br_3NO_2$		7*A10 + 4*A12 + A11 + A4*B4 + 3*A25 + 2*A50 + A32 3,5-dibromo-N-(4-bromophenyl)-2-hydroxybenzamide				

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
497.7	28.67	0	57.6	74.0	28.67	36.8
$\text{C}_{13}\text{H}_8\text{Cl}_2\text{O}$	$6^*A10+6^*A12+3^*A21+A31+A60$ <i>p, p'</i> -dichlorobenzophenone					[221]
420	30.12	0	71.71	66.3	30.12	27.9
$\text{C}_{13}\text{H}_8\text{O}$	$2^*A22^*C22+A35+8^*A10+4^*A12$ xanthene					[215]
373.7	19.2	0	51.38	56.0	19.2	20.9
$\text{C}_{13}\text{H}_8\text{O}$	$A14+3^*A15+2^*A19+8^*A10+A112+2^*A19$ 9-fluorenone					[215]
356.4	18.12	0	50.84	49.7	18.12	17.7
$\text{C}_{13}\text{H}_8\text{OS}$	$8^*A10+A14+2^*A15+2^*A19+A114+2^*A19$ thioxanthone					[215]
487.9	35.5	0	72.76	56.3	35.5	27.5
$\text{C}_{13}\text{H}_8\text{O}_2$	$A14+3^*A15+4^*A19+A114+A131+8^*A10$ xanthone					[160]
449.7	26.12	0	58.08	54.6	26.12	24.6
$\text{C}_{13}\text{H}_9\text{Cl}_3\text{N}_2\text{O}$	$A14+3^*A15+4^*A19+A112+A114+8^*A10$ benzoic acid, 2,4,6-trichlorophenyl hydrazide					[216]
439.7	32.71	0	74.4	59.2	32.71	26.0
$\text{C}_{13}\text{H}_9\text{F}_3\text{N}_2\text{O}_2$	$7^*A10+5^*A12+3^*A22^*D22+A60+A44$ 2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid					[221]
476	38	0	79.83	72.8	38	34.6
$\text{C}_{13}\text{H}_9\text{N}$	$3^*A25+A4^*B4+7^*A10+3^*A12+A11+A44+A41+A36$ acridine					[85]
383.2	18.58	0	48.48	47.7	18.58	18.3
$\text{C}_{13}\text{H}_9\text{N}$	$9^*A10+2^*A12+A41+2^*A12$ 7,8-benzoquinoline					[284]
324.1	14.1	0	43.51	47.7	14.1	15.5
$\text{C}_{13}\text{H}_9\text{N}$	$9^*A10+4^*A12+A41$ phenanthridine					[216]
354	0.02	0.06				
379.7	22.83	60.12	60.18	47.7	22.85	18.1
$\text{C}_{13}\text{H}_9\text{N}_2$	$9^*A10+4^*A12+A41$ 2-phenylbenzimidazole					[216]
572.2	22.18	0	38.75	65.9	22.18	37.7
$\text{C}_{13}\text{H}_{10}$	$9^*A10+A118+A121+A14+2^*A15+3^*A19+A12$ fluorene					
387.9	19.58	0	50.48	51.0	19.58	19.8
$\text{C}_{13}\text{H}_{10}\text{BrCl}_2\text{O}_2\text{PS}$	$8^*A10+A14+2^*A15+4^*A19$ O-(4-bromo-2,5-dichlorophenyl)O-methyl phenylphosphonothioate					[216]
345.6	31.35	0	90.73	87.2	31.35	30.1
$\text{C}_{13}\text{H}_{10}\text{Cl}_2\text{S}$	$7^*A10+5^*A12+A1+2^*A22^*D22+A21+A81$ <i>p</i> -chlorobenzyl <i>p</i> -chlorophenyl sulfide					[221]
343.8	32.22	0	93.71	68.9	32.22	23.7
$\text{C}_{13}\text{H}_{10}\text{N}_2$	$8^*A10+3^*A12+A11+2^*A22^*D22+A2+A84$ diphenylcarbodiimide					[232]
287.4	18.55	0	64.54	52.9	18.55	15.2
$\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}$	$10^*A10+2^*A12+2^*A42+A9$ 1,3-diphenylurea					[227]
512	34.6	0	67.58	60.7	34.6	31.1
$\text{C}_{13}\text{H}_{10}\text{O}$	$10^*A10+2^*A12+A66$ benzophenone					[215]
321.0	18.19	0	56.67	63.8	18.19	20.5
$\text{C}_{13}\text{H}_{10}\text{S}$	$10^*A10+2^*A12+A35$ thioxanthene					[80]
401.8	26.1	0	64.96	57.6	26.1	23.2
$\text{C}_{13}\text{H}_{11}\text{N}$	$A14+3^*A15+2^*A19+2^*A19+A131+8^*A10$ N-methylcarbazole					[215]
362.5	17.15	0	47.32	49.3	17.15	17.9
$\text{C}_{13}\text{H}_{11}\text{NO}$	$A14+2^*A15+2^*A19+2^*A19+A119+A1+8^*A10$ benzanilide					[216]
436.5	29.61	0	67.84	60.6	29.61	26.5
$\text{C}_{13}\text{H}_{12}$	$10^*A10+2^*A12+A60$ diphenylmethane					[216]
298.3	18.58	0	62.34	62.1	18.58	18.5
	$10^*A10+A2+2^*A11$					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$C_{13}H_{12}NO$	1,3-diphenylurea 34.62	0	67.6	60.7	34.62	31.1
	$10^*A10+2^*A12+A66$					[216]
$C_{13}H_{12}O$	diphenylcarbinol 23	0	67.93	46.9	23	15.9
	$10^*A10+2^*A11+A3^*B3+A30$					[216]
$C_{13}H_{13}BrS$	2- <i>n</i> -propyl-5-(4-bromophenyl)thiophene 15.7	0	43.56	58.7	15.7	21.2
	$A14+2^*A15+A131+2^*A19+2^*A19+A1+2+4^*A10+2^*A12+A21$					[251]
$C_{13}H_{13}N$	N-benzylaniline 16.76	0	54.84	85.6	16.76	26.2
	$10^*A10+A12+A11+A45+A2$					[215]
$C_{13}H_{13}NO_2$	(<i>dl</i>) 2-(1-naphthoxy)propionamide 37.66	0	84.62	69.8	37.66	31.1
	$7^*A10+3^*A12+A32+A3^*B3+A1+A61$					[273]
$C_{17}H_{13}NO_2$	(<i>d</i>) 2-(1-naphthoxy)propionamide 38.07	0	80.16	69.8	38.07	33.2
	$7^*A10+2^*A12+A32+A3^*B3+A1+A61+A12$					[273]
$C_{13}H_{14}N_2$	<i>bis</i> -(4-aminophenyl)methane 9.23	0	25.36	75.0	9.23	27.3
	$8^*A10+2^*A11+2^*A12+2^*A45+A2$					[216]
$C_{13}H_{15}N$	1,2,3,4-tetrahydro-9-methylcarbazole 0.08	0.5				
	14.67	45.29	45.8	39.2	14.75	12.7
	$2^*A14+3^*A15+2^*A19+2^*A19+4^*A10+A119$					[15]
$C_{13}H_{15}NO_2$	3,4-dihydro-6-methyl-2H-pyran-5-carboxanilide 19.21	0	50.4	69.8	19.21	26.6
	$A14+3^*A15+A112+2^*A19+A60+5^*A10+A12+A1$					[221]
$C_{13}H_{15}N_3O_2$	3-methyl-1-phenyl-1H-pyrazol-5-yl dimethylcarbamate 21.39	0	65.96	65.9	21.39	21.4
	$A14+2^*A15+3^*A1+5^*A10+A12+A68+3^*A19+A12+A118$					[221]
$C_{13}H_{16}F_3N_3O_4$	2,6-dinitro- <i>N,N</i> -dipropyl-4-(trifluoromethyl)benzenamine 22.32	0	69.45	76.6	22.32	24.6
	$2^*A10+A11+3^*A12+2^*A50+A43+3^*A25$ $+A4^*B4+2^*A1+4^*A2$					[215]
$C_{13}H_{16}F_3N_3O_4$	<i>N</i> -butyl- <i>N</i> -ethyl-2,6-dinitro-4-trifluoromethylaniline 36.5	0	107.83	76.6	36.5	25.9
	$2^*A10+A11+3^*A12+2^*A50+A43+3^*A25+A4^*B4+2^*A1+4^*A2$					[215]
$C_{13}H_{18}$	1,1,4,6-tetramethylindane 15.74	0	57.53	47.6	15.74	13.0
	$4^*A1+2^*A10+2^*A11+A14+2^*A15+A17+2^*A19$					[215]
$C_{13}H_{18}$	1,1,4,7-tetramethylindane 11.28	0	45.93	47.6	11.28	11.7
	$4^*A1+2^*A10+2^*A11+A14+2^*A15+A17+2^*A19$					[215]
$C_{13}H_{18}ClNO$	<i>N</i> -(4-chlorophenyl)-2,2-dimethylpentanamide 23.31	0	64.71	76.5	23.31	27.6
	$3^*A1+2^*A2+A4^*B4+4^*A10+2^*A12+A22^*B22+A60$					[221]
$C_{13}H_{18}ClNO$	<i>N</i> -(3-chloro-4-methylphenyl)-2-methylpentanamide 16.35	0	46.28	72.6	16.35	25.6
	$3^*A1+2^*A2+2^*A12+A11+A3^*B3+3^*A10+A60+A22^*B22$					[221]
$C_{13}H_{18}N_2O_2$	3-cyclohexyl-6,7-dihydro-1H-cyclopentapyrimidine-2,4-(3H,5H)-dione 42.31	0	72.41	64.0	42.31	37.4
	$3^*A14+6^*A15+A16+A124+A125+2^*A19$					[221]
$C_{13}H_{18}O_5S$	<i>dl</i> -2-ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranyl methanesulfonate 26.25	0	76.28	68.3	26.25	23.5
	$A14+2^*A15+A19+A17+A16+A122+4^*A1+A2+3^*A10+A12+A89$					[221]
$C_{13}H_{19}NO_2$	hexyl <i>N</i> -phenylcarbamate 32.76	0	100	93.4	32.76	30.7
	$5^*A10+A12+A1+5^*A2+A69$					[102]
$C_{13}H_{19}N_3O_4$	<i>N</i> -(1-ethylpropyl)-2,6-dinitro-3,4-xylylidine 25.19	0	76.92	70.7	25.19	23.1
	$4^*A1+2^*A2+A3^*B3+A44+2^*A50+3^*A12+2^*A11+A10$					[215]
$C_{13}H_{21}N_2O$	<i>N,N</i> -dimethyl- <i>N'</i> -(octahydro-4,7-methano-1H-inden-5-yl)urea 21.74	0	49.81	65.5	21.74	28.6
	$3^*A14+A15+5^*A16+2^*A1+A64$					[221]
$C_{13}H_{22}$	1,3,5-trimethyladamantane 6.3	27.61				

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
253.6	1.73	6.82	34.43	38.2	8.03	9.7
$C_{13}H_{22}O_3$	$3*A14+A15+A16+3*A17+3*A1$ 3,3,7,7-tetramethylnonanedioic anhydride					[146]
396.2	20.5	0	51.75	62.8	20.5	24.9
$C_{13}H_{24}N_6$	$A14+7*A15+4*A1+2*A17+A117$ 1-(hexamethyleneimine)-3,5-bis(dimethylamino)-s-triazine					[109]
335.8	16.32	0	48.6	65.0	16.32	21.8
$C_{13}H_{24}O_2$	$A14*4*A15+A119+4*A1+2*A43+3*A12+3*A41$ tridecanolactone					[242]
290.6	18.16	62.37				
300.4	9.08	30.21	92.55	77.2	27.24	23.2
$C_{13}H_{24}O_4$	$A14+11*A15+A115$ tridecanedioic acid					[216]
387.5	45.3	0	116.9	134.9	45.3	52.3
$C_{13}H_{26}$	$11*A2*B2+2*A36*B36$ cyclotridecane					[216]
285.6	0.9	3.15				
297.6	7.4	24.87	28.02	70.4	8.3	20.9
$C_{13}H_{26}$	$A14+10*A15$ <i>n</i> -heptylcyclohexane					[181]
232.8	22.22	0	95.43	90.1	22.22	21.0
$C_{13}H_{26}O_2$	$A14+A16+A1+6*A2+3*A15$ tridecanoic acid					[216]
307.1	8.72	28.41				
315.0	33.74	107.11	135.52	133.6	42.47	42.1
$C_{13}H_{26}O_2Si_3$	$11*A2*B2+A1+A36$ 1,1,1,3,5,5,5-heptamethyl-3-phenyltrisiloxane					[216]
226.8	18.29	0	80.64	80.8	18.29	18.3
$C_{13}H_{27}NO_2$	$7*A1+5*A10+A12+2*A32+3*A109$ 3(<i>n</i> -nonylamino)-1,2-propanediol					[216]
343.2	53.2	0	155.01	125.5	53.2	43.1
$C_{13}H_{28}$	$A1+8*A2*B2+A44+2*A30*C30+A3*B3+2*A2$ <i>n</i> -tridecane					[217]
255	7.66	30.04				
267.8	28.49	106.27	136.31	137.8	36.15	36.9
$C_{13}H_{28}O$	$2*A1+11*A2*B2$ tri- <i>tert</i> -butylmethanol					[216]
302	7.2	23.84				
390	3.43	8.379	32.64	32.6	10.63	12.7
$C_{13}H_{28}O$	$9*A1+3*A4+A30+A4*B4$ tridecanol					[216]
304.6	45.1					
304.5	41.42	138.9				
303.5	23.3	76.99				
301.6	3.6	12.13				
305.8	22.09	72.38				
306.6	18.74	61.09	148.11	131.3	45.02	40.3
$C_{13}H_{28}O_2S$	$A1+12*A2*B2+A30$ 3(<i>n</i> -decylthio)-1,2-propanediol					[224]
291.9	17.3	59.27				
311.9	17.3	55.47	114.73	142.3	34.6	44.4
$C_{13}H_{28}O_2$	$A1+9*A2*B2+A84+2*A30*C30+A3*B3+2*A2$ 3(<i>n</i> -decyloxy)-1,2-propanediol					[217]
311	38.9	0	125.08	144.9	38.9	45.1
$C_{13}H_{29}NO_2$	$A1+9*A2*B2+A32+2*A30*C30+A3*B3+2*A2$ 3(<i>n</i> -decylamino)-1,2-propanediol					[217]
346.6	54.8	0	158.11	134.9	54.8	46.8
$C_{14}H_7ClF_3NO_5$	$A1+9*A2*B2+A44+2*A30*C30+2*A2+A3*B3$ 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoic acid					[217]
436.6	37.67	0	86.27	83.0	37.67	36.2
$C_{14}H_7ClO_2$	$6*A10+A11+5*A12+A22*G22+A36*F36+A32+A50+A4*B4+3*A25$ 2-chloroanthraquinone					[221]
483.0	39	0	80.74	53.3	39	25.7
$C_{14}H_8Cl_4$	$A14+3*A15+4*A19+2*A114+A22*C22+A12+7*A10$ 1-chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl)benzene					[216]
349.8	23.84	0	68.17	72.7	23.84	25.4
$C_{14}H_8Cl_4$	$8*A10+4*A12+A7+A7+4*A22*D22$ 1,1-dichloro-2,2-bis(4-chlorophenyl)ethylene					[221]
360.4	23.55	0	65.33	72.7	23.55	26.2
	$8*A10+4*A12+A7+A7+4*A22*D22$					[221]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{14}H_8O_2$	anthraquinone					
555	32.57	0	58.7	52.0	32.57	29.0
	3*A15+A14+8*A10+4*A19+2*A114					[216]
$C_{14}H_9ClF_2N_2O_2$	N-[[4-chlorophenylamino]carbonyl]-2,6-difluorobenzamide					
499.5	55.99	0	112.08	66.8	55.99	33.4
	7*A10+5*A12+2*A24+A22*E22+2*A60					[221]
$C_{14}H_9Cl_2NO_3$	methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate					
358.3	26.31	0	73.44	79.7	26.31	28.5
	6*A10+6*A12+2*A22*E22+A50+A32+A38+A1					[215]
$C_{14}H_9Cl_3$	1-chloro-2,2-(bis-(4-chlorophenyl)ethylene					
337.9	25.52	0	75.53	71.2	25.52	24.0
	8*A10+4*A12+A6*B6+A7+3*A22*C22					[232]
$C_{14}H_9Cl_5$	1,1-(2,2,2-trichloroethylidene)bis(4-chlorobenzene)					
382.1	26.28	0	68.78	66.9	26.28	25.5
	5*A22*E22+A4*B4+2*A12+2*A11+8*A10+A3					[215]
$C_{14}H_9Cl_5$	1-chloro-2-(2,2,2-trichloro-1-(4-chlorophenyl)ethyl)benzene					
345.8	23.09	0	66.78	66.9	23.09	23.1
	8*A10+2*A12+2*A11+5*A22*E22+A3+A4*B4					[221]
$C_{14}H_9Cl_5O$	2-chloro- α -(4-chlorophenyl)- α -(trichloromethyl)benzenemethanol					
396.3	25.2	0	63.61	83.1	25.2	32.9
	8*A10+2*A11+2*A12+2*A4*B4+5*A22*F22+A30*F30					[215]
$C_{14}H_9Cl_5O$	4-chloro- α -(4-chlorophenyl)- α -(trichloromethyl)benzenemethanol					
347.2	19.56	0	56.35	83.1	19.56	28.9
	8*A10+2*A11+2*A12+2*A4*B4+5*A22*F22+A30*F30					[221]
$C_{14}H_9NO_4PS$	O-ethyl O-(4-nitrophenyl)phenylphosphonothioate					
308.2	25.05	0	81.29	91.9	25.05	28.3
	9*A10+3*A12+A50+A1+A2+A81					[221]
$C_{14}H_9NO_2$	1-aminoanthraquinone					
524.2	28.78	0	54.9	58.5	28.78	30.7
	A14+3*A15+2*A114+4*A19+7*A10+A45+A12					[13]
$C_{14}H_{10}$	phenanthrene					
347.5	0.22	0.63				
372.4	16.46	44.21	44.83	44.2	16.68	16.5
	10*A10+4*A12					[216]
$C_{14}H_{10}$	anthracene					
488.9	29.37	0	60.08	44.2	29.37	21.6
	10*A10+4*A12					[216]
$C_{14}H_{10}$	diphenylacetylene					
334	20.5	0	61.4	53.7	20.5	17.9
	10*A10+2*A9+2*A12					
$C_{14}H_{10}Cl_2O_2$	bis(4-chlorophenyl)acetic acid					
440.2	31.66	0	71.92	77.7	31.66	34.2
	8*A10+2*A12+2*A11+A3*B3+2*A22*C22+A36*C36					[215]
$C_{14}H_{10}Cl_4$	1,1'-(2,2-dichloroethylidene)bis(4-chlorobenzene)					
382.1	27.31	0	71.48	63.9	27.31	24.4
	8*A10+2*A11+2*A12+A3*B3+4*A22*D22					[215]
$C_{14}H_{10}N_2O_2$	1,4-diaminoanthraquinone					
484.2	24.2	0	49.98	65.0	24.2	31.5
	A14*3*A15+2*A114+4*A19+6*A10+2*A45+2*A12					[13]
$C_{14}H_{10}O$	anthrone (some decomposition upon melting)					
429	26.8	0	62.47	53.4	26.8	22.9
	A14+3*A15+2*A19+2*A19+8*A10+A114					[82]
$C_{14}H_{10}O_2$	benzil					
84	0.04	0.5				
368	23.56	64.02	64.52	68.4	23.6	25.2
	10*A10+2*A12+2*A35					[216]
$C_{14}H_{10}O_3$	benzoic anhydride					
313.2	17.15	0	54.77	69.2	17.15	21.7
	10*A10+2*A12+A39					[287]
$C_{14}H_{11}Cl_2NO_2$	3-(3,5-dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3.1.0]hexanedione					
438.2	30.09	0	68.67	66.1	30.09	29.0
	2*A14+A128+2*A17+3*A12+2*A22*C22+2*A1					[221]
$C_{14}H_{11}NO_3$	N-salicylidene- <i>m</i> -aminobenzoic acid					
464	33.11	0	71.36	77.9	33.11	36.2
	8*A10+4*A12+A36*C36+A31+A42+A6*B6					[216]
$C_{14}H_{12}$	9,10-dihydrophenanthrene					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
306.5	12.8	0	41.77	54.7	12.8	16.8
$C_{14}H_{12}$	8*A10+A14+3*A15+4*A19 <i>trans</i> -stilbene					[216]
398.2	27.4	0	68.81	69.7	27.4	27.8
$C_{14}H_{12}$	10*A10+2*A12+2*A6 9-methylfluorene					[215]
319.2	16.32	0	51.13	53.9	16.32	17.2
$C_{14}H_{12}F_3NO_4S_2$	A14+2*A15+4*A19+A16+A1+8*A10 1,1,1-trifluoro- <i>n</i> -[2-methyl-4-(phenylsulphonyl)phenyl]methane sulfonamide					[252]
418.4	31.79	0	75.97	68.7	31.79	36.0
$C_{14}H_{12}O_2$	8*A10+A11+3*A12+A88+A95+A4*B4+3*A25+A1 diphenylacetic acid					[221]
420.4	31.25	0	74.34	58.7	31.25	24.7
$C_{14}H_{12}O_2$	10*A10+2*A11+A3*B3+A36 benzyl benzoate					[216]
293.1	20.44	0	69.76	71.9	20.44	21.1
$C_{14}H_{12}O_4$	10*A10+A11+A12+A2+A38 1,2-dicarbomethoxynaphthalene					[221]
358.2	27.6	0	77.05	65.1	27.6	23.3
$C_{14}H_{12}O_4$	6*A10+4*A12+2*A1+2*A38 1,3-dicarbomethoxynaphthalene					[217]
378.7	30.5	0	80.54	65.1	30.5	24.64
$C_{14}H_{12}O_4$	6*A10+2*A12+2*A1+2*A38+2*A12 1,4-dicarbomethoxynaphthalene					[217]
340.2	20.4	0	59.96	65.1	20.4	22.13
$C_{14}H_{12}O_4$	6*A10+2*A12+2*A1+2*A38+2*A12 1,5-dicarbomethoxynaphthalene					[217]
392	26.4	0	67.35	65.1	26.4	25.5
$C_{14}H_{12}O_4$	6*A10+2*A12+2*A1+2*A38+2*A12 1,6-dicarbomethoxynaphthalene					[217]
371.8	22.1	0	59.44	65.1	22.1	24.2
$C_{14}H_{12}O_4$	6*A10+2*A12+2*A1+2*A38+2*A12 1,7-dicarbomethoxynaphthalene					[217]
363.2	20	0	55.07	65.1	20	23.6
$C_{14}H_{12}O_4$	6*A10+2*A12+2*A1+2*A38+2*A12 2,3-dicarbomethoxynaphthalene					[217]
324.2	20.2	0	62.31	65.1	20.2	21.1
$C_{14}H_{12}O_4$	6*A10+2*A12+2*A1+2*A38+2*A12 2,7-dicarbomethoxynaphthalene					[217]
410.2	26.6	0	64.85	65.1	26.6	26.7
$C_{14}H_{14}$	6*A10+2*A12+2*A1+2*A38+2*A12 1,2,3,4-tetrahydrophenanthrene					[217]
302.6	11.17	36.91				
285	5.83	20.44				
298	1.77	5.92	63.28	49.5	18.76	14.7
$C_{14}H_{14}$	A14+3*A15+2*A19+2*A12+6*A10 phenyl- <i>o</i> -tolylmethane					[31]
279.8	19.24	0	68.78	62.6	19.24	17.5
$C_{14}H_{14}^*$	9*A10+3*A11+A1+A2 2,2'-dimethylbiphenyl					[216]
293.1	2.28	0	7.78	0	2.28	0
$C_{14}H_{14}$	Prediction not made 1,2-diphenylethane					[216]
273.2	2.25	8.23				
324.3	22.73	70.09	78.32	69.2	24.98	22.4
$C_{14}H_{14}^*$	10*A10+2*A11+2*A2 2-ethylbiphenyl					[216]
267.1	2.07	0	7.74	0	2.07	0
$C_{14}H_{14}$	Prediction not made 1,2,3,4-tetrahydroanthracene					[216]
373.3	19.16	51.33				
388	2.92	7.53	58.85	49.5	22.08	19.2
$C_{14}H_{14}Cl_2N_2O$	A14+3*A15+2*A19+6*A10+2*A12 1-[2-(2,4-dichlorophenyl)-2-(propenyloxy)ethyl]-1H-imidazole					[216]
322.6	30.5	0	94.55	74.5	30.5	24.0
	A14+2*A15+3*A18*B18+A119+A118+2*A2+A3*B3+A5+A6 +3*A10+2*A12+A11+2*A22*E22+A32					[221]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$C_{14}H_{14}NO_4PS$	O-ethyl O-(4-nitrophenyl)phenylphosphonothioate					
308.2	25.05	0	81.28	74.2	25.05	22.9 [221]
$C_{14}H_{14}O_2$	9*A10+3*A12+A1+A2+A81 (dl) 1,2-diphenyl-1,2-dihydroxyethane					
393	31.38	0	79.85	71.9	31.38	28.2 [273]
$C_{14}H_{14}O_2$	10*A10+2*A11+2*A3*B3+2*A30*B30 (d) 1,2-diphenyl-1,2-dihydroxyethane					
420.5	34.31	0	81.59	71.9	34.31	30.2 [273]
$C_{14}H_{14}O_3$	10*A10+2*A11+2*A3*B3+2*A30*B30 2-(6-methoxy-2-naphthyl)propionic acid					
439.2	29.41	0	66.96	58.6	29.41	25.7 [33]
$C_{14}H_{14}O_3$	6*A10+3*A12+A11+2*A1+A3*B3+A36*B36+A32 2-pivaloylindan-1,3-dione					
381.5	25.99	0	68.12	62.9	25.99	24.0 [215]
$C_{14}H_{15}N_3$	A14+2*A15+2*A19+2*A114+4*A10+3*A1+A4*B4+A35+A16 N,N-dimethyl-4-phenylazoaniline					
389.2	23.08	0	59.3	53.7	23.08	20.9 [13]
$C_{14}H_{16}$	2*A1+A43+9*A10+3*A12+2*A42 heptacyclo[6.6.0[2.6].0[3,13].0[4,11].0[5,9].0[8,1].O[10,14]]tetradecane					
355	14.67	41.32				
440	5.57	12.66	53.98	31.0	20.24	13.6 [127]
$C_{14}H_{16}ClN_3O_2$	7*A14-7*A15+12*A16 1-(4-chlorophenoxy)-3,3-dimethyl-(1H,1,2,4-triazol-1-yl)-2-butanone					
351.4	22.87	0	65.06	76.6	22.87	26.9 [221]
$C_{14}H_{16}F_3N_3O_4$	4*A10+2*A12+3*A1+A4*B4+A3*B3+A14+2*A15+2*A18*B18 +2*A118+A22*F22+A119+A35+A32 N-(cyclopropylmethyl)-2,6-dinitro- <i>n</i> -propyl-4-(trifluoromethyl)benzenamine					
305.8	22.51	0	73.61	70.9	22.51	21.7 [221]
$C_{14}H_{16}O_8$	3*A12+2*A10+A11+A4*B4+3*A25+2*A50+A43+A1+3*A2+A14+A16 1,2,3,4-tetracarboxymethoxybenzene					
404.7	40.4	0	99.79	85.9	40.4	34.8 [217]
$C_{14}H_{16}O_8$	4*A1+4*A38+4*A12+2*A10 1,2,3,5-tetracarboxymethoxybenzene					
389.2	32.6	0	83.89	85.9	32.6	33.4 [217]
$C_{14}H_{16}O_8$	4*A1+4*A38+4*A12+2*A10 1,2,4,5-tetracarboxymethoxybenzene					
416.7	35.7	0	85.4	85.9	35.7	35.8 [217]
$C_{14}H_{17}ClNPO_4S_2$	4*A1+4*A38+4*A12+2*A10 S-[2-chloro-1-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]O,O-diethylphosphorodithioate					
340.0	25.27	0	74.33	101.1	25.27	34.4 [221]
$C_{14}H_{17}NO_2$	A14+2*A15+2*A19+4*A10+A128+4*A2+2*A1+A80 4-methyl-7-diethylaminocoumarin					
343.8	17.88	0	52.02	67.2	17.88	23.1 [216]
$C_{14}H_{18}$	A14+3*A15+2*A19+A19+A18*B18+A115+3*A10+A12+3*A1+2*A2+A43 1,2,3,4,5,6,7,8-octahydroanthracene					
331.4	2.51	7.59				
345.4	18.34	53.1	60.69	54.7	20.86	18.9 [216]
$C_{14}H_{18}ClN_3O_2$	2*A14+6*A15+4*A19+2*A10 β (4-chlorophenoxy)- α -(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol					
377.8	24.47	0	64.77	73.0	24.47	27.6 [221]
$C_{14}H_{19}Cl_2NO_2$	A14+2*A15+2*A118+A119+2*A18*B18+2*A3*B3 +A32+A22*F22+4*A10+2*A12+3*A1+A4+A30*F30 4[<i>p</i> -[bis(2-chloroethyl)amino]benzene]butanoic acid					
338.9	29.18	0	86.1	102.7	29.18	34.8 [221]
$C_{14}H_{19}NO$	3*A2+4*A2+4*A10+A11+A12+A36*D36+2*A22*D22+A4 2-(dimethylamino)-1,2-diphenylethanone					
334.2	22.38	0	66.97	64.7	22.38	21.6 [253]
$C_{14}H_{20}$	10*A10+A11+A12+A35*B35+A43+2*A1+A3*B3 diamantane					
407.2	4.44	10.89				
440.4	8.95	20.33				
517.9	8.66	16.72	47.95	45.4	22.05	23.5 [216]
$C_{14}H_{20}$	5*A14-A15+8*A16 1,8-cyclotetradecadiyne					
370	22.6	0	61.06	55.3	22.6	20.4 [108]
	A14+11*A15+4*A20					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
$C_{14}H_{20}O$	1-diamantanol					
408	4.9	12.01				
395	18	45.57				
573	9.6	16.75	74.33	27.3	32.5	15.6
	$5^*A14 - A15 + 7^*A16 + A17 + A30$					[144]
$C_{14}H_{20}O$	4-diamantanol					
448	9.77	21.81				
484	16.4	33.88	55.69	27.3	26.17	13.2
	$5^*A14 - A15 + 7^*A16 + A17 + A30$					[144]
$C_{14}H_{20}ClNO_2$	2-chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide					
315.9	25.31	0	80.13	86.5	25.31	27.3
	$3^*A1 + 4^*A2 + 3^*A10 + 2^*A11 + A12 + A32 + A22^*C22 + A59$					[221]
$C_{14}H_{20}N_3O_5PS$	O-6-ethoxycarbonyl-5-methylpyrazolo[1,5- <i>a</i>]pyrimidin-2-yl O,O-diethyl phosphorothioate					
324.4	27.32	0	84.22	97.6	27.32	31.66
	$A14 + 2^*A15 + A18 + 2^*A19 + A118 + A119 + A10 + A11 + A12 + A41 + A38 + 4^*A1 + 3^*A2 + A79$					[221]
$C_{14}H_{21}N_3O_4$	4-(1,1-dimethylethyl)- <i>n</i> -(1-methylpropyl)-2,6-dinitrobenzamine					
338.8	20.84	0	61.52	63.5	20.84	21.5
	$2^*A10 + A11 + 3^*A12 + 5^*A1 + A4 + A2 + A3^*B3 + 2^*A50 + A44$					[221]
$C_{14}H_{22}$	<i>n</i> -octylbenzene					
234.2	29.96	0	127.91	110.4	29.96	25.9
	$A1 + 7^*A2^*B2 + 5^*A10 + A11$					[216]
$C_{14}H_{22}N_4O_2$	8-heptyltheophylline					
472.7	33	0	69.81	95.9	33	45.3
	$2^*A14 + 3^*A15 + 2^*A125 + A118 + A121 + 3^*A1 + 3^*A1 + 3^*A19 + 6^*A2$					[216]
$C_{14}H_{22}N_4O_6S$	4-(dipropylamino)-N,N-dimethyl-3,5-dinitrobenzenesulfonamide					
413.6	32.57	0	78.75	85.7	32.57	35.4
	$4^*A1 + 4^*A2 + A43 + 2^*A50 + A94 + 2^*A10 + 4^*A12$					[221]
$C_{14}H_{22}O$	2,6-di- <i>tert</i> -butylphenol					
310.7	16.57	0	53.33	51.6	16.57	16.0
	$6^*A1 + 2^*A4 + 2^*A11 + A12 + 3^*A10 + A31$					[101]
$C_{14}H_{24}$	1,3,5,7-tetramethyladamantane					
183.3	0.23	1.25				
337.2	9.82	29.12	30.38	35.9	10.05	12.1
	$3^*A14 + A15 + 4^*A17 + 4^*A1$					[146]
$C_{14}H_{24}$	<i>cis</i> -anti- <i>trans</i> -perhydrophenanthrene					
313	11.16	0	35.64	59.7	11.16	18.7
	$3^*A14 + 5^*A15 + 4^*A16$					[216]
$C_{14}H_{24}$	<i>cis</i> -syn- <i>trans</i> -perhydrophenanthrene					
273	10.48	0	38.39	59.7	10.48	16.3
	$3^*A14 + 5^*A15 + 4^*A16$					[216]
$C_{14}H_{24}$	<i>trans</i> -anti- <i>trans</i> -perhydrophenanthrene					
283	11.83	0	41.81	59.7	11.83	16.9
	$3^*A14 + 5^*A15 + 4^*A16$					[216]
$C_{14}H_{24}O_2$	1,8-cyclotetradecanedione					
417.2	27.53	0	65.99	71.4	27.53	29.8
	$A14 + 11^*A15 + 2^*A114$					[114]
$C_{14}H_{24}NO_4PS_3$	O,O-diisopropyl S-2-phenylsulfonylaminoethyl phosphorodithioate					
310.4	30.61	0	98.63	91.2	30.61	28.3
	$5^*A10 + A12 + 2^*A2 + 4^*A1 + 2^*A3^*B3 + A95 + A80$					[221]
$C_{14}H_{24}O_4$	1,6-cyclodecanedione bis ethylene ketal					
450.2	32.68	0	72.58	69.2	32.68	31.2
	$3^*A14 + 9^*A15 + 4^*A112 + 2^*A17$					[114]
$C_{14}H_{26}O$	4,4,8,8-tetramethylcyclodecanone					
378.2	16.32	0	43.15	59.1	16.32	22.4
	$A14 + 7^*A15 + 4^*A1 + 2^*A17 + A114$					[111]
$C_{14}H_{26}O_2$	decyl methacrylate					
250.7	30.55	0	121.85	133.4	30.55	33.5
	$2^*A1 + 9^*A2^*B2 + A5 + A7 + A38$					[216]
$C_{14}H_{28}$	cyclotetradecane					
328	28.7	0	87.51	74.1	28.7	24.3
	$11^*A15 + A14$					[119]
$C_{14}H_{28}O$	2-tetradecanone					
306.7	49.12	0	160.16	142.4	49.12	43.7
	$2^*A1 + A35 + 11^*A2^*B2$					[216]
$C_{14}H_{28}O_2$	ethyl dodecanoate					
271.5	9.31	0	34.3	0	9.31	
	Prediction not made					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C ₁₄ H ₂₈ O ₂	327	tetradecanoic acid	0	137.92	45.1	46.7
		12*A2*B2+A1+A36				
C ₁₄ H ₂₈ O ₄	409.4	2,2,9,9-tetramethyl-1,3,8,10-tetraoxacyclotetradecane	0	74.5	80.1	32.8
		A14+11*A15+4*A112+4*A1+2*A17				
C ₁₄ H ₂₉ NO ₃	393.1	N-dodecylglycine	0	123.12	138.2	54.3
		A1+11*A2*B2+A2+A36*B36+A44				
C ₁₄ H ₂₉ NO ₃	357.1 398.1	N-octyl-L-leucine	21.28 73.6	94.88	110.0	36.9
		3*A1+7*A2*B2+A3+A3*B3+A36*B36+A44+A2				
C ₁₄ H ₂₉ NO ₃	353.6 367.1	N-octyl-DL-leucine	19.23 74.09	93.33	110.0	34.0
		3*A1+7*A2*B2+A3+A3*B3+A36*B36+A44+A2				
C ₁₄ H ₃₀	279	tetradecane	0	161.54	147.1	45.07
		2*A1+12*A2*B2				
C ₁₄ H ₃₀ O	311.2 310.8 306 311 311.6 311	1-tetradecanol	151.04 80.75 5.86 76.57 70.71 158.75	140.6	49.37	43.7
		47.01				
		25.1				
		1.8				
		23.81				
		22.01				
		49.37				
A1+13*A2*B2+A30	[224]					
C ₁₄ H ₃₀ O ₂ S	280.2 289.1 295.2 317.4	3(<i>n</i> -undecylthio)-1,2-propanediol	8.92 16.95 15.58 57.66	99.11	151.6	30.3
		2.5				
		4.9				
		4.6				
A1+10*A2*B2+A84+2*A30*C30+2*A2+A3*B3	[217]					
C ₁₄ H ₃₀ O ₃	311.7	3(<i>n</i> -undecyloxy)-1,2-propanediol	0	138.27	154.2	43.1
		43.1				
C ₁₄ H ₃₁ NO ₂	348.8	3(<i>n</i> -undecylamino)-1,2-propanediol	0	166.86	144.2	58.2
		58.2				
C ₁₅ H ₁₀ N ₂ O ₂	313.6	4,4'-diphenylmethane diisocyanate	0	87.06	78.5	27.3
		27.3				
C ₁₅ H ₁₁ ClF ₃ NO ₄	358.8	2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene	0	83.8	82.4	30.07
		30.07				
C ₁₅ H ₁₁ ClN ₂ O	216.7	6*A10+A11+5*A12+A1+A2+A4*B4+3*A25+A22*G22+A50+2*A32	0	156.9	69.7	34
		7-chloro-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one				
C ₁₅ H ₁₂	182 295 324.9	A14+4*A15+2*A121+A22*C22+A16+A19+A18+5*A10+A12	0.12 0.11 43.21	43.44	44.8	14.09
		4-methylphenanthrene				
		0.02				
		0.03				
C ₁₅ H ₁₂ N ₂ O ₃	515.2	A1+9*A10+4*A12+A11	0	68.5	72.4	32.29
		1,4-diamino-2-methoxyanthraquinone				
C ₁₅ H ₁₃ Cl ₂ NO ₂	354.3	A14+3*A15+2*A114+4*A19+5*A10+2*A45+3*A12+A1+A32	0	60.38	66.8	21.39
		1,1-(di- <i>p</i> -chlorophenyl)-2-nitropropane				
C ₁₅ H ₁₄ O	307.2	8*A10+2*A11+2*A12+A3+A3*B3+A1+2*A22*C22+A50	0	65.77	73.8	20.2
		1,3-diphenylacetone				
C ₁₅ H ₁₅ ClN ₂ O ₂	425.8	10*A10+2*A11+2*A2+A35	0	81.88	82.9	34.87
		3-[4-[4-chlorophenoxy]phenyl]-1,1-dimethylurea				
C ₁₅ H ₁₅ N	137.5 180	8*A10+4*A12+2*A1+A22*C22+A32*C32+A64*B64	4.64 2.09			35.3
		N-isopropylcarbazole				

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)	
395.2	17.73	44.86	51.6	57.2	18.75	22.6	
$C_{15}H_{15}NO$	A 14 + 2*A 15 + 2*A 19 + 8*A 10 + 2*A 1 + A 3*B 3 + A 119 + 2*A 19 N-methylidiphenylacetamide						[142]
439.8	30.23	0	68.73	64.3	30.23	28.3	
$C_{15}H_{16}N_2O_2$	10*A 10 + 2*A 11 + A 3*B 3 + A 1 + A 60 <i>a</i> -cyclopropyl- <i>a</i> -(4-methoxyphenyl)-5-pyrimidinemethanol						[221]
383.1	26.63	0	69.51	88.0	26.63	33.7	
$C_{15}H_{16}O$	A 14 + 7*A 10 + A 1 + A 4*B 4 + 2*A 11 + A 12 + 2*A 41 + A 30*D 30 + A 32 + A 16 <i>p</i> - α -cumylphenol						[221]
346.4	21.68	0	62.58	66.3	21.68	23.0	
$C_{15}H_{16}O_2$	8*A 10 + 3*A 12 + A 11 + 2*A 1 + A 3 + A 31 4,4'-dihydroxydiphenyl-2,2-propane						[216]
433	30.1	0	69.52	66.0	30.1	28.6	
$C_{15}H_{17}Br_2NO_2$	2*A 1 + A 4 + 8*A 10 + 2*A 12 + 2*A 11 + 2*A 31 3,5-dibromo-4-hydroxybenzoxazole octanoyl ester						[216]
318.3	26.49	0	83.23	105.8	26.49	33.7	
$C_{15}H_{18}Cl_2N_2O_3$	4*A 12 + 2*A 10 + 2*A 21 + A 56 + A 38 + A 1 + 6*A 2 3-[2,4-dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)- 1,3,4-oxadiazol-2(3H)-one						[221]
360.6	26.39	0	73.19	89.3	26.39	32.2	
$C_{15}H_{18}N_2O_6$	A 14 + 2*A 15 + A 19 + A 126 + A 118 + 5*A 1 + A 3*B 3 + A 4 + 4*A 12 + 2*A 10 + 2*A 22*E 22 + A 32 2-sec-butyl-4,6-dinitrophenyl 3-methylcrotonate						[221]
341.3	18.89	0	55.37	80.2	18.89	27.4	
$C_{15}H_{21}NO$	4*A 1 + A 2 + A 3 + 2*A 10 + 3*A 12 + A 11 + 2*A 50 + A 38 + A 7 + A 6*B 6 2-methyl-1-phenyl-2-(N-piperidinyl)-1-propanone						[222]
310.2	16.74	0	53.97	71.7	16.74	22.2	
$C_{15}H_{21}NO_4$	5*A 10 + A 12 + A 4*B 4 + 2*A 1 + A 14 + 3*A 15 + A 119 + A 35 methyl N-(2-methoxyacetyl)-N-(2,6-xylyl)-dl-alaninate						[254]
345.5	26.46	0	76.58	82.1	26.46	28.4	
$C_{15}H_{23}N_3O_2$	5*A 1 + A 2 + A 3*B 3 + 3*A 10 + 2*A 11 + A 12 + A 38 + A 32 + A 59 N-capryl-pyrazinamide						[221]
360.5	50.58	0	140.31	104.7	50.58	37.7	
$C_{15}H_{24}O$	A 1 + 6*A 2 + 3*A 10 + A 12 + 2*A 41 + A 71 2,6-di- <i>tert</i> -butyl-4-methylphenol						[9]
343.7	23.85	0	69.39	52.2	23.85	17.9	
$C_{15}H_{24}O_2$	7*A 1 + 2*A 10 + 3*A 11 + A 12 + 2*A 4 + A 31 2,6-di- <i>tert</i> -butyl-4-methoxyphenol						[101]
374.4	26.9	0	71.86	59.0	26.9	22.1	
$C_{15}H_{28}O_2$	7*A 1 + 2*A 4 + 2*A 11 + 2*A 12 + 2*A 10 + A 31 + A 32 pentadecanolactone						[114]
283	27.3	96.47					
308.5	6.99	22.65	119.12	84.6	34.29	26.1	
$C_{15}H_{30}$	A 14 + 13*A 15 + A 115 cyclopentadecane						[282]
210.1	8.5	40.46					
336.6	8.5	25.25	65.71	77.8	17	26.2	
$C_{15}H_{30}$	A 14 + 12*A 15 <i>n</i> -decylcyclopentane						[181]
251.0	33.14	0	132.01	127.6	33.14	32.0	
$C_{15}H_{30}O$	A 14 + A 16 + A 1 + 9*A 2*B 2 + 2*A 15 2-pentadecanone						[216]
312.2	54.57	0	174.8	151.7	54.39	47.4	
$C_{15}H_{30}O_2$	2*A 1 + A 35 + 12*A 2*B 2 pentadecanoic acid						[216]
318.7	8.12	25.48					
325.7	41.52	127.49	152.97	152.3	49.64	49.6	
$C_{15}H_{30}O_2$	13*A 2*B 2 + A 1 + A 36 methyl myristate						[216]
291.6	50.21	0	172.17	154.8	50.21	45.1	
$C_{15}H_{31}NO_3$	2*A 1 + 12*A 2*B 2 + A 38 N-decyl-L-valine						[217]
378.1	21.3	56.33					
380.6	15.4	40.46	96.8	121.5	36.7	46.3	
$C_{15}H_{31}NO_3$	3*A 1 + A 3 + A 3*B 3 + 9*A 2*B 2 + A 44 + A 36*B 36 N-decyl-DL-valine						[249]
358.1	63.1	0	176.21	121.5	63.1	43.5	

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)	
$C_{15}H_{31}NO_3$	356.1	3*A1+A3+A3*B3+9*A2*B2+A44+A36*B36 N-dodecyl-L-alanine		105.59	139.0	[249]	
		37.6	0			37.6	49.5
$C_{15}H_{32}$	270.9 283.1	2*A1+11*A2*B2+A3*B3+A36*B36+A44 <i>n</i> -pentadecane		156.02	156.5	[249]	
		9.17	33.85			43.77	44.3
		34.6	122.17			43.77	44.3
$C_{15}H_{32}O$	316 316.6	2*A1+13*A2*B2 1-pentadecanol		172.8	150.0	[216]	
		23.64	74.81			54.73	47.5
$C_{15}H_{32}O_2S$	299 325.5	A1+14*A2*B2+A30 3(<i>n</i> -dodecylthio)-1,2-propanediol		122.9	160.9	[224]	
		18.1	60.54			18.1	52.4
$C_{15}H_{32}O_3$	323	A1+11*A2*B2+A84+2*A30*C30+2*A2+A3*B3 3(<i>n</i> -dodecyloxy)-1,2-propanediol		159.13	163.5	[217]	
		20.3	62.37			51.4	52.8
$C_{15}H_{33}NO_2$	351.9	A1+11*A2*B2+A32+2*A30*C30+2*A2+A3*B3 3(<i>n</i> -dodecylamino)-1,2-propanediol		176.47	153.5	[217]	
		62.1	0			62.1	54.0
$C_{16}F_{34}$	176.5 177.7 186.7 402.2	A1+11*A2*B2+A44+2*A30*C30+2*A2+A3*B3 perfluorohexadecane		185.35	172.0	[217]	
		1.13	6.4			67.12	69.2
		3.01	16.94			67.12	69.2
		1.89	10.12			67.12	69.2
$C_{16}H_{10}$	120.8 423.8	16*A4*B4+6*A25+28*A26 pyrene		43.36	43.8	[67]	
		0.29	2.39			17.65	18.6
$C_{16}H_{10}$	383.4	10*A10+4*A12+2*A13 1,2-benzacenaphthene (fluoranthene)		48.89	36.5	[216]	
		18.74	0			18.74	14.0
$C_{16}H_{11}F_3O$	356.8	10*A10+5*A12+A13 4-ethoxy-2',3',4'-trifluorodiphenylacetylene		90.25	73.4	[216]	
		32.2	0			32.2	26.2
$C_{16}H_{12}F_2$	301.2	6*A10+6*A12+2*A9+A2+A1+3*A24+A32 4-ethyl-3',4'-difluorodiphenylacetylene		55.11	64.8	[196]	
		16.6	0			16.6	19.5
$C_{16}H_{12}F_2O$	343.4	7*A10+A11+4*A12+2*A9+A2+A1+2*A24 4-ethoxy-2',4'-difluorodiphenylacetylene		78.63	71.64	[196]	
		27	0			27	24.6
$C_{16}H_{13}FO$	354.4	7*A10+5*A12+2*A9+A2+A1+2*A24+A32*C32 4-ethoxy-4'-fluorodiphenylacetylene		64.33	69.9	[196]	
		22.8	0			22.8	24.8
$C_{16}H_{12}Ge$	320	8*A10+4*A12+2*A9+A2+A1+A24*B24+A32 diphenyldiethynylgermane		62.81	48.3	[196]	
		20.1	0			20.1	15.5
$C_{16}H_{12}Si$	316.2	10*A10+2*A12+2*A8+2*A9+A102 diphenyldiethynylsilane		62.21	52.2	[48]	
		19.67	0			19.67	16.5
$C_{16}H_{14}$	319.9 385.1 412.8	10*A10+2*A11+2*A8+2*A9+A109 4,5,9,10-tetrahydropyrene		47.53	52.5	[216]	
		1.85	5.77			19.07	21.7
		0.13	0.34			19.07	21.7
		17.09	41.41			19.07	21.7
$C_{16}H_{14}Cl_2O_3$	310.4	2*A14+4*A15+6*A19+6*A10 ethyl 2-hydroxy-2,2-bis-(4-chlorophenyl)acetate		75.64	90.0	[18]	
		23.48	0			23.48	27.9
$C_{16}H_{14}Cl_2O_4$	314.4	8*A10+2*A11+2*A12+A1+A2+A4*B4+2*A22*D22+A30*D30+A38 methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate		86.13	89.3	[215]	
		27.08	0			27.08	28.1
$C_{16}H_{14}O_2$	187 418.6	7*A10+5*A12+2*A1+A3*B3+A38+2*A32+2*A22*D22 1,2-dibenzoylthane		94.56	82.6	[221]	
		0.22	1.17			39.21	34.6
		38.99	93.3			39.21	34.6
		10*A10+2*A12+2*A2+2*A35				[216]	

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (calcd)
$C_{16}H_{14}O_6$	1,2,3-tricarbomethoxynaphthalene					
362.7	23.7	0	65.34	75.4	23.7	27.4
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	1,2,4-tricarbomethoxynaphthalene					
393.7	32.1	0	81.53	75.4	32.1	29.7
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	1,2,5-tricarbomethoxynaphthalene					
363	25.5	0	70.25	75.4	25.5	27.4
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	1,2,6-tricarbomethoxynaphthalene					
416.7	35.9	0	86.15	75.4	35.9	31.4
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	1,2,7-tricarbomethoxynaphthalene					
427.2	36.1	0	84.5	75.4	36.1	32.2
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	1,2,8-tricarbomethoxynaphthalene					
366.7	24.8	0	67.63	75.4	24.8	27.7
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	1,3,5-tricarbomethoxynaphthalene					
402.7	25.9	0	64.35	75.4	25.9	30.4
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	1,3,7-tricarbomethoxynaphthalene					
446.7	37.2	0	83.39	75.4	37.2	33.7
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	1,3,8-tricarbomethoxynaphthalene					
388.2	27.7	0	71.46	75.4	27.7	29.3
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	1,4,5--tricarbomethoxynaphthalene					
402.2	26.5	0	65.77	75.4	26.5	30.3
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	1,4,6-tricarbomethoxynaphthalene					
409.2	30.2	0	73.6	75.4	30.2	30.9
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	2,3,5-tricarbomethoxynaphthalene					
401.7	41	0	101.96	75.4	41	30.3
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{14}O_6$	2,3,6-tricarbomethoxynaphthalene					
399.2	34.4	0	86.27	75.4	34.4	30.1
	$3^*A1 + 3^*A38 + 2^*A12 + 5^*A10 + 3^*A12$					[217]
$C_{16}H_{15}Cl_2NO_2$	1,1-bis(4-chlorophenyl)-2-nitrobutane					
330.3	15.41	0	46.65	73.8	15.41	24.4
	$8^*A10 + 2^*A12 + 2^*A11 + A3 + A3^*B3 + A1 + A2 + 2^*A22^*C22 + A50$					[221]
$C_{16}H_{15}Cl_3O_2$	1-methoxy-2-(2,2,2-trichloro-1(4-methoxyphenyl)ethyl)benzene					
347.6	22.45	0	64.58	85.6	22.45	29.8
	$8^*A10 + 2^*A12 + 2^*A11 + 2^*A1 + A4^*B4 + 2^*A32 + 3^*A22^*E22 + A3^*B3$					[221]
$C_{16}H_{15}Cl_3O_2$	1,1'-(2,2,2-trichloroethylidene-bis(4-methoxy)benzene					
360.6	27.48	76.14	76.21	85.6	27.48	30.9
	$8^*A10 + 2^*A12 + 2^*A11 + 2^*A1 + A4^*B4 + 2^*A32 + 3^*A22^*E22 + A3^*B3$					[221]
$C_{16}H_{15}N$	4'-propylbiphenyl-4-carbonitrile					
338.8	22.7	0	67.01	76.8	22.7	26.0
	$A1 + 2^*A2 + 8^*A10 + A11 + 3^*A12 + A56$					[216]
$C_{16}H_{16}$	1,2,3,6,7,8-hexahydropyrene					
377	5.02	13.32				
407.7	18.09	44.37	57.69	45.0	23.11	18.4
	$2^*A14 + 6^*A15 + 6^*A19 + 4^*A10$					[18]
$C_{16}H_{16}N_2O_2^*$	anisaldazine					
442	29.75	0	67.31	0	29.75	0
	No prediction made					[216]
$C_{16}H_{16}N_2O_4$	ethyl [3-[[[(phenylamino)carbonyl]oxy]phenyl]carbamate					
394.1	32.75	0	83.09	90.2	32.75	35.6
	$9^*A10 + 3^*A12 + 2^*A69 + A1 + A2$					[221]
$C_{16}H_{16}N_2O_4$	methyl 3- <i>m</i> -tolylcarbamoyloxphenylcarbamate					
423.8	39.62	0	93.49	83.6	39.62	35.4
	$2^*A1 + 3^*A12 + A11 + 8^*A10 + 2^*A69$					[221]
$C_{16}H_{16}O_2$	(<i>d</i>) 2-(<i>p</i> -methoxyphenyl)propiophenone					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)	
326	21.76	0	66.74	76.8	21.76	25.0	
$C_{16}H_{16}O_2$	9*A10+2*A12+A3*B3+2*A1+A32+A11+A35 (dl) 2-(<i>p</i> -methoxyphenyl)propionophenone						[273]
353	26.36	0	74.67	76.8	26.36	27.1	
$C_{16}H_{16}O_3$	9*A10+2*A12+A3*B3+2*A1+A32+A11+A35 2,2-dimethoxy-1,2-diphenylethanone						[273]
338.5	20.86	0	61.63	83.4	20.86	28.2	
$C_{16}H_{17}NO$	10*A10+A11+A12+2*A1+2*A32*C32+A35+A4*B4 N,N-dimethyl-2,2-diphenylacetamide						[28]
407.1	25.43	67.55	62.47	69.3	25.43	28.2	
$C_{16}H_{18}FN_3O_3$	2*A1+10*A10+2*A11+A3*B3+A59 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic acid						[217]
500.2	32.97	0	65.91	82.5	32.97	41.3	
$C_{16}H_{18}N_2O^*$	2*A14+6*A15+2*A119+A121+A114+3*A19 +A18*B18+2*A12+2*A10+A24+A36+A1+A2 4- <i>n</i> -butyl-4'-hydroxyazobenzene						[36]
351.6	5.25	0	14.93	0	5.25	0	
$C_{16}H_{18}N_4O_4$	No prediction made N,N-(2-hydroxyethyl)-4-(4-nitrophenyl)azoaniline						[131]
484.2	32.43	0	66.97	92.1	32.43	44.6	
$C_{16}H_{19}BrO_2$	8*A10+4*A12+4*A2+2*A30*E30+2*A42+A43+A50 4- <i>trans</i> -(4-bromophenyl)cyclohexyl (E)-2-butenolate						[13]
388.2	28.4	0	73.16	79.6	28.4	30.9	
$C_{16}H_{19}ClO_2$	A14+3*A15+2*A16+4*A10+A11+A12+A21+A38 +A1+A6*B6+A6 4- <i>trans</i> -(4-chlorophenyl)cyclohexyl (E)-2-butenolate						[140]
386.2	30.2	0	78.2	78.2	30.2	30.2	
$C_{16}H_{19}FO_2$	A14+3*A15+2*A16+4*A10+A11+A12+A38 +A1+A6*B6+A6+A22*B22 4- <i>trans</i> -(4-fluorophenyl)cyclohexyl (E)-2-butenolate						[140]
354.2	25.1	0	70.86	78.6	25.1	27.9	
$C_{16}H_{19}N_3O_2$	A14+3*A15+2*A16+4*A10+A11+A12+A38+A1+A6*B6+A6+A24 N,N-(2-hydroxyethyl)-4-phenylazoaniline						[140]
407	29.96	0	73.61	89.3	29.96	36.3	
$C_{16}H_{20}N_2$	9*A10+3*A12+4*A2+2*A30*E30+2*A42+A43 tetracyclopropylsuccinonitrile						[13]
390	22.3	0	57.18	64.4	22.3	25.1	
$C_{16}H_{20}O_6P_2S_3$	4*A14+4*A16+2*A4*B4+2*A56 O,O,O',O'-tetramethyl O,O'-thiodi- <i>p</i> -phenylene bis(phosphorothioate)						[216]
303.2	33.03	0	108.94	104.0	33.03	31.5	
$C_{16}H_{22}NClO_3$	8*A10+4*A12+A84+2*A79+4*A1 N-(chloroacetyl)- <i>n</i> -(2,6-diethylphenyl)glycine ethyl ester						[221]
318	23.84	0	74.97	96.6	23.84	30.7	
$C_{16}H_{22}O_3Si_3$	3*A1+5*A2+3*A10+2*A11+A12+A22*C22+A59+A38 1,1,3,3-tetramethyl-5,5-diphenylcyclotrisiloxane						[221]
338.0	22.19	0	65.66	69.3	22.19	23.4	
$C_{16}H_{24}N_6$	4*A1+A14+3*A15+3*A112+3*A139+10*A10+2*A11 1-(methylphenethylamino)-3,5-bis(dimethylamino)- <i>s</i> -triazine						[216]
334.2	20.04	0	59.96	73.2	20.04	24.5	
$C_{16}H_{25}NO_2$	5*A1+2*A2+A11+5*A10+3*A41+3*A12+3*A43 nonyl phenylcarbamate						[215]
327	28.07	0	85.77	132.4	28.07	43.3	
$C_{16}H_{28}O_2$	5*A10+A12+A1+8*A2*B2+A69 1,9-cyclohexadecanedione						[102]
301.2	17.95	59.59					
351.2	8.03	22.87	82.47	78.8	25.98	27.7	
$C_{16}H_{28}O_4$	A14+13*A15+2*A114 1,7-cyclododecanedione bis ethylene ketal						[114]
478.2	36.94	0	77.26	76.6	36.94	36.6	
$C_{16}H_{32}$	3*A14+11*A15+2*A17+4*A112 cyclohexadecane						[114]
271.2	18.83	69.42					
283.2	1.26	4.43					
332.2	4.18	12.59	86.45	81.5	24.27	27.1	
$C_{16}H_{32}$	A14+13*A15 <i>n</i> -decylcyclohexane						[112]
271.4	38.62	0	142.29	131.3	38.62	35.6	

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
						[215]
$C_{16}H_{32}$	$9*A2*B2 + A1 + A14 + 3*A15 + A16$					
	1-hexadecene					
249.2	3.87	15.53				
277.5	30.21	108.86	124.39	161.5	34.08	44.8
	$A5 + A6 + 13*A2*B2 + A1$					[165]
$C_{16}H_{32}O_2$	hexadecanoic acid					
335.7	54.81	0	163.27	161.6	54.81	54.2
	$14*A2*B2 + A1 + A36$					[216]
$C_{16}H_{32}O_4$	6,6,14,14-tetramethyl-1,3,9,11-tetraoxacyclohexadecane					
358.6	29.71	0	82.84	87.5	29.71	31.4
	$A14 + 13*A15 + 4*A112 + 4*A1 + 2*A17$					[117]
$C_{16}H_{32}O_4$	2,2,10,10-tetramethyl-1,3,9,11-tetraoxacyclohexadecane					
371.3	25.94	0	69.87	87.5	25.94	32.5
	$A14 + 13*A15 + 4*A112 + 4*A1 + 2*A17$					[117]
$C_{16}H_{32}O_8$	1,4,7,10,13,16,19,22-octaoxacyclotetracosane					
292.2	34.5	0	118.07	118.4	34.5	34.6
	$A14 + 21*A15 + 6*A112$					[120]
$C_{16}H_{33}NO$	N-hexyl decanamide					
301	6	19.93				
311	31	99.68	119.61	157.9	37	49.1
	$2*A1 + 13*A2*B2 + A60$					[127]
$C_{16}H_{33}NO$	N-butyl dodecanamide					
322.1	39	0	121.08	151.0	39.0	48.7
	$2*A1 + 10*A2*B2 + A60 + 3*A2$					[127]
$C_{16}H_{33}NO_3$	N-tetradecylglycine					
379.6	6.8	17.91				
396.6	47.4	119.52	137.43	156.8	54.2	62.2
	$13*A2*B2 + A1 + A44 + A36*B36 + A2$					[249]
$C_{16}H_{33}NO_3$	N-decyl-L-leucine					
343.1	1.2	3.5				
383.1	27.5	71.78	75.28	128.7	28.7	49.3
	$3*A1 + 9*A2*B2 + A3 + A3*B3 + A36*B36 + A44 + A2$					[249]
$C_{16}H_{33}NO_3$	N-decyl-DL-leucine					
357.1	28.9	0	71.78	128.7	28.9	45.9
	$3*A1 + 9*A2*B2 + A3 + A3*B3 + A36*B36 + A44 + A2$					[249]
$C_{16}H_{34}$	hexadecane					
291.3	53.35	183.13				
291.1	51.46	176.79	176.79	165.8	53.35	48.3
	$2*A1 + 14*A2*B2$					[216]
$C_{16}H_{34}O$	1-hexadecanol					
322.3	33.6	104.18				
322.2	23.72	73.22				
322.2	58.41	181.17	181.17	159.3	58.41	51.3
	$A1 + 15*A2*B2 + A30$					[224]
$C_{16}H_{34}O_2S$	3(<i>n</i> -tridecylthio)-1,2-propanediol					
296.9	11.3	38.06				
330.6	22.7	68.66	106.72	170.3	34	56.3
	$A1 + 12*A2*B2 + A84 + 2*A30*C30 + 2*A2 + A3*B3$					[217]
$C_{16}H_{34}O_3$	3(<i>n</i> -tridecyloxy)-1,2-propanediol					
342.2	51.4	0	158.54	172.9	51.4	56.0
	$A1 + 12*A2*B2 + A32 + 2*A30*C30 + 2*A2 + A3*B3$					[217]
$C_{16}H_{35}NO_2$	3(<i>n</i> -tridecylamino)-1,2-propanediol					
354.9	68.7	0	193.58	162.9	68.7	57.8
	$A1 + 12*A2*B2 + A44 + 2*A30*C30 + 2*A2 + A3*B3$					[217]
$C_{16}H_{36}Ge$	tetrabutylgermane					
198.6	19.1	0	96.17	120.8	19.1	24.0
	$4*A1 + 12*A2 + A102$					[53]
$C_{16}H_{40}O_4Si_4$	octaethylcyclotetrasiloxane					
208.2	12.22	58.7				
213.4	13.71	64.24	122.94	115.7	25.92	24.7
	$8*A1 + 8*A2 + 4*A112 + 4*A139 + A14 + 5*A15$					[227]
$C_{17}H_{12}$	1,2-benzofluorene					
399.9	3.8	9.5				
462.8	18.4	39.76	49.26	50.9	22.2	23.6
	$A14 + 2*A15 + 4*A19 + 10*A10 + 2*A12$					[216]
$C_{17}H_{12}$	2,3-benzofluorene					
489.7	23.4	0	47.78	50.9	23.4	24.9
	$A14 + 2*A15 + 4*A19 + 10*A10 + 2*A12$					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C ₁₇ H ₁₂ O	371.2	4-ethynyl-1-[(4-ethynylphenyl)methoxy]benzene 21.2	0	57.11	21.2	23.5
		2*A9+2*A8+3*A12+A11+A2+A32+8*A10				[216]
C ₁₇ H ₁₂ O ₂	440.6	4-benzoyl-1-naphthol 28.64	0	65	28.64	30.4
		11*A10+5*A12+A35+A31				[215]
C ₁₇ H ₁₂ O ₂	414.1	1-benzoyl-2-naphthol 31.35	0	75.71	31.35	28.6
		11*A10+5*A12+A35+A31				[215]
C ₁₇ H ₁₂ O ₂	343.9	2-benzoyl-1-naphthol 20.18	0	58.68	20.18	23.7
		11*A10+5*A12+A35+A31				[215]
C ₁₇ H ₁₂ O ₂	329.2	1-naphthyl benzoate 16.98	0	51.58	16.98	22.0
		12*A10+4*A12+A38				[118]
C ₁₇ H ₁₂ O ₂	381.2	2-naphthyl benzoate 26.23	0	68.81	26.23	25.4
		12*A10+4*A12+A38				[118]
C ₁₇ H ₁₃ F ₃ O	327.3	4- <i>n</i> -propoxy-2',3',4'-trifluorodiphenylacetylene 26.1	0	79.74	26.1	26.4
		6*A10+6*A12+3*A24+2*A2+A1+2*A9+A32				[196]
C ₁₇ H ₁₄ F ₂	311	4- <i>n</i> -propyl-3',4'-difluorodiphenylacetylene 20.2	0	64.95	20.2	22.4
		7*A10+A11+4*A12+2*A24+2*A2+A1+2*A9				[196]
C ₁₇ H ₁₄ F ₂ O	326.9	4- <i>n</i> -propoxy-2',4'-difluorodiphenylacetylene 25.2	0	77.09	25.2	25.8
		7*A10+5*A12+2*A24+2*A2+A1+2*A9+A32				[196]
C ₁₇ H ₁₄ N ₂ O ₂	355.8	2,2-bis-(4-cyanatophenyl)propane 26.69	0	75.02	26.69	25.51
		2*A1+A4+2*A11+2*A12+2*A58+8*A10				[216]
C ₁₇ H ₁₄ O ₅	391.8	3-[1-(2-furanyl)-3-oxobutyl]-4-hydroxy-2H-1-benzopyran-2-one 33.88	0	86.49	33.88	34.3
		2*A14+5*A15+5*A19+2*A18+A18*B18+4*A10+A1 +A2+A3+A35+A115+A112+A30*D30				[221]
C ₁₇ H ₁₅ F	324	4- <i>n</i> -propyl-4'-fluorodiphenylacetylene 24.1	0	74.38	24.1	22.8
		8*A10+A11+3*A12+A24+2*A2+A1+2*A9				[196]
C ₁₇ H ₁₅ FO	356.8	4- <i>n</i> -propoxy-4'-fluorodiphenylacetylene 27.1	0	75.95	27.1	27.5
		8*A10+4*A12+A24+2*A2+A1+2*A9+A32				[196]
C ₁₇ H ₁₆ Br ₂ O ₃	348.1	isopropyl 4,4'-dibromobenzilate 24.55	0	70.53	24.55	32.5
		8*A10+2*A11+2*A12+A30*D30+A38+2*A1+A3*B3+2*A21+A4*B4				[216]
C ₁₇ H ₁₈ FN ₃ O ₃	541.5	1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3- quinolinecarboxylic acid 64.48	0	119.08	64.48	49.4
		3*A14+6*A15+3*A19+A18*B18+A114+2*A119 +A121+2*A10+2*A12+A36*F36+A24				[36]
C ₁₇ H ₁₉ FNO ₂	393.2	4- <i>trans</i> -(3-fluoro-4-cyanophenyl)cyclohexyl (E)-but-2-enoate 21.1	0	53.66	21.1	32.0
		3*A10+2*A12+A11+A24+A56+A14+3*A15+2*A16+A38+A6+A6*B6+A1				[140]
C ₁₇ H ₁₉ F ₃ O ₃	340.2	4- <i>trans</i> -(trifluoromethoxyphenyl)cyclohexyl (E)-but-2-enoate 21.6	0	63.49	21.6	28.4
		4*A10+A12+A11+3*A25+A14+3*A15+2*A16 +A38+A6+A6*B6+A1+A32+A4*B4				[140]
C ₁₇ H ₂₁ NO ₂	345.3	N,N-diethyl-2-(1-naphthoxy)propionamide 24.57	0	71.16	24.57	27.7
		3*A1+2*A2+B3*A3+7*A10+3*A12+A32+A59				[221]
C ₁₇ H ₃₄ O	323.9	9-heptadecanone 66.68	0	205.87	66.68	55.2
		2*A1+A35+A14*A2*B2				[21]
C ₁₇ H ₃₄ O ₂	329.2	heptadecanoic acid 7.44	22.59			
	334.3	51.33	153.55	176.15	170.9	57.1
C ₁₇ H ₃₄ O ₂		15*A2*B2+A1+A36				[216]
		methyl palmitate				
C ₁₇ H ₃₄ O ₂	307.2	68.16	0	221.84	68.16	53.3
	305.2	55.35		181.4	55.35	

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
	$2*A1 + 14*A2*B2 + A38$					[217, 391]
$C_{17}H_{35}NO_3$	N-tetradecyl-L-alanine					
367.1	52.3	0	142.47	157.6	52.3	57.9
	$2*A1 + 13*A2*B2 + A3*B3 + A44 + A36*B36$					[249]
$C_{17}H_{35}NO_3$	N-dodecyl-L-valine					
380.1	33.1	0	87.08	140.2	33.1	53.3
	$3*A1 + A3 + A3*B3 + 11*A2*B2 + A44 + A36*B26$					[249]
$C_{17}H_{35}NO_3$	N-dodecyl-DL-valine					
364.6	64.4	0	176.63	140.2	64.4	51.1
	$3*A1 + A3 + A3*B3 + 11*A2*B2 + A44 + A36*B36$					[249]
$C_{17}H_{36}$	<i>n</i> -heptadecane					
284.3	10.96	38.56				
295.1	40.17	136.11	174.67	175.1	51.13	51.7
	$2*A1 + 15*A2*B2$					[216]
$C_{17}H_{36}O_2S$	3(<i>n</i> -tetradecylthio)-1,2-propanediol					
302.5	16.3	53.88				
336.4	26.8	79.67	133.55	179.6	43.1	60.4
	$A1 + 13*A2*B2 + A84 + 2*A30*C30 + 2*A2 + A3*B3$					[217]
$C_{17}H_{36}O_3$	3(<i>n</i> -tetradecyloxy)-1,2-propanediol					
331.3	62.1	0	187.44	182.2	62.1	60.4
	$A1 + 13*A2*B2 + A32 + 2*A30*C30 + 2*A2 + A3*B3$					[217]
$C_{17}H_{37}NO_2$	3(<i>n</i> -tetradecylamino)-1,2-propanediol					
356.2	64.9	0	182.2	172.2	64.9	61.3
	$A1 + 13*A2*B2 + A32 + 2*A30*C30 + 2*A2 + A3*B3$					[217]
$C_{18}H_{10}$	benzofluoranthene					
402.8	5.35	13.28				
402.1	0.88	2.19				
352.7	0.44	1.23				
424	11.8	27.83	44.53	36.1	18.47	15.3
	$10*A10 + 5*A12 + 3*A13$					[264]
$C_{18}H_{12}$	triphenylene					
471	24.74	0	52.53	44.1	24.74	20.8
	$12*A10 + 6*A12$					[216]
$C_{18}H_{12}$	chrysene					
512.2	3.22	6.29				
531.4	26.15	49.21	55.5	44.1	29.37	23.4
	$12*A10 + 6*A12$					[255]
$C_{18}H_{12}$	1,2-benzanthracene					
434.3	21.38	0	49.23	44.1	21.38	19.1
	$12*A10 + 6*A12$					[215]
$C_{18}H_{12}$	3,4-benzophenanthrene					
334.7	16.32	0	48.75	44.1	16.32	14.8
	$12*A10 + 6*A12$					[215]
$C_{18}H_{13}FO$	4-ethoxy-4'-fluorodiphenyldiacetylene					
400.2	33.9	0	84.71	64.4	33.9	25.8
	$A1 + A2 + 4*A12 + 8*A10 + 4*A9 + A24*B24 + A32$					[195]
$C_{18}H_{14}$	<i>m</i> -terphenyl					
360	22.59	0	62.76	73.9	22.59	26.6
	$14*A10 + 4*A12$					[256]
$C_{18}H_{14}$	<i>p</i> -terphenyl					
193.6	0.3	1.6				
487	35.3	72.5	74.1	73.9	35.6	35.9
	$14*A10 + 4*A12$					[38,155]
$C_{18}H_{14}$	<i>o</i> -terphenyl					
329.4	17.2	0	52.3	73.9	17.2	24.3
	$14*10 + 4*A12$					[91]
$C_{18}H_{14}O_3$	cinnamic anhydride					
321.2	32.77	0	102.02	87.6	32.77	28.1
	$10*A10 + 2*A12 + A39 + 2*A6 + 2*A6*B6$					[215]
$C_{18}H_{15}F_3O$	4- <i>n</i> -butoxy-1',3',4'-trifluorodiphenylacetylene					
344.4	36	0	104.53	87.7	36	30.2
	$6*A10 + 6*A12 + 3*A24 + A32 + 3*A2 + A1 + 2*A9$					[196]
$C_{18}H_{15}ClSi$	triphenylchlorosilane					
370.6	26.88	0	72.53	77.9	26.88	28.9
	$15*A10 + 3*A12 + A109 + A22*B22$					[216]
$C_{18}H_{15}N$	triphenylamine					
400.2	24.89	0	62.21	66.5	24.89	26.6
	$15*A10 + 3*A12 + A43$					[217]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C ₁₈ H ₁₅ OP 431.9	triphenylphosphine oxide 24.22	0	56.08	56.1	24.22	24.2
	15*A10+3*A12+A73					[246]
C ₁₈ H ₁₅ O ₄ P 322.5	triphenyl phosphate 29.61	0	91.81	78.8	29.61	25.4
	15*A10+3*A12+A74					[215]
C ₁₈ H ₁₅ P 354.4	triphenylphosphine 19.69	0	55.56	68.0	19.69	24.1
	15*A10+3*A12+A72					[246]
C ₁₈ H ₁₆ F ₂ 323.5	4- <i>n</i> -butyl-3',4'-difluorodiphenylacetylene 25.3	0	78.21	79.1	25.3	25.6
	7*A10+A11+4*A12+2*A24+3*A2+A1+2*A9					[196]
C ₁₈ H ₁₆ O ₃ 371.2	1,8-diphenyl-2,3,5-trioxabicyclo[4.3.0]non-7-ene 21.7	0	58.46	45.3	21.7	16.8
	10*A10+A11+A12+2*A14+3*A15+A19+A18+6*A16 +A17+A112+A113					[257]
C ₁₈ H ₁₆ O ₈ 423.7	1,2,3,4-tetracarboxynaphthalene 35.9	0	84.47	85.8	35.9	36.3
	4*A1+4*A38+4*A10+6*A12					[217]
C ₁₈ H ₁₆ O ₈ 438.2	1,2,4,5-tetracarboxynaphthalene 36.4	0	82.89	85.8	36.4	37.6
	4*A1+4*A38+4*A10+6*A12					[217]
C ₁₈ H ₁₆ O ₈ 470.2	1,2,5,6-tetracarboxynaphthalene 42.1	0	89.37	85.8	42.1	40.3
	4*A1+4*A38+4*A10+6*A12					[217]
C ₁₈ H ₁₆ O ₈ 407.2	1,2,6,7-tetracarboxynaphthalene 34.2	0	83.76	85.8	34.2	34.9
	4*A1+4*A38+4*A10+6*A12					[217]
C ₁₈ H ₁₆ O ₈ 458.2	2,3,6,7-tetracarboxynaphthalene 42.2	0	91.88	85.8	42.2	39.3
	4*A1+4*A38+4*A10+6*A12					[217]
C ₁₈ H ₁₆ O ₈ 477.2	1,4,5,8-tetracarboxynaphthalene 36.1	0	75.69	85.8	36.1	40.9
	4*A1+4*A38+4*A10+6*A12					[217]
C ₁₈ H ₁₇ Cl ₂ NO ₃ 341.7	ethyl <i>N</i> -benzoyl- <i>n</i> -(3,4-dichlorophenyl)- <i>dl</i> -alaninate 27.06	0	79.19	90.9	27.06	31.1
	8*A10+4*A12+2*A1+A2+A3*B3+A38+2*A22*D22+A59					[221]
C ₁₈ H ₁₇ F 329.9	4- <i>n</i> -butyl-4'-fluorodiphenylacetylene 18.5	0	56.08	77.4	18.5	25.5
	8*A10+A11+3*A12+A24+3*A2+A1+2*A9					[196]
C ₁₈ H ₁₇ FO 346.7	4- <i>n</i> -butoxy-4'-fluorodiphenylacetylene 25.4	0	73.26	84.2	25.4	29.4
	8*A10+4*A12+A24+3*A2+A1+2*A9+A32					[196]
C ₁₈ H ₁₈ 369	1-methyl-7-isopropylphenanthrene 18.03	0	48.87	46.6	18.03	17.2
	8*A10+3*A1+2*A11+A3+4*A12					[216]
C ₁₈ H ₁₈ CINS 370.3	2-chloro-9-(3-dimethylaminopropylidene)-10-thioxanthene 27.82	0	75.13	77.8	27.82	28.8
	A14+3*A15+2*A19+38*A19+A131+7*A10+A12+A22*C22+A6*B6 +2*A2+2*A1+A43					[216]
C ₁₈ H ₁₈ N ₂ O ₂ 521.2	<i>N,N'</i> -(2-hydroxyethyl)-1,4-diaminoanthraquinone 32.34	0	62.05	86.0	32.34	44.8
	A14+3*A15+2*A114+4*A19+6*A10+2*A44+2*A12+4*A2+2*A30*D30					[13]
C ₁₈ H ₁₈ O ₂ 387.2	3-diphenylmethyl-2,4-pentanedione 27.02	0	69.78	73.3	27.02	28.4
	2*A1+A3*B3+2*A35+A3+10*A10+2*A11					[259]
C ₁₈ H ₁₈ O ₃ 343.9	butyl 9-hydroxy-9H-fluorene-9-carboxylate 25.56	0	74.31	81.2	25.56	27.9
	A14+2*A15+8*A10+4*A19+A17+A30*B30+A38+A1+3*A2					[215]
C ₁₈ H ₂₀ Cl ₂ 331.6	1,1'-(2,2-dichloroethylidene)bis(4-ethylbenzene) 23.34	0	70.38	76.7	23.34	25.4
	8*A10+4*A11+A3+A3*B3+2*A1+2*A2+2*A22*B22					[215]
C ₁₈ H ₂₀ O ₂ 443.8 441.8	diethylstilbestrol 31.76	0	71.57	97.8	31.76	43.5
	8*A10+4*A12+2*A31+2*A7+2*1+2*A2					[221, 394]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
$C_{18}H_{22}$	2,3-dimethyl-2,3-diphenylbutane					
392	25.52	0	65.11	55.6	25.52	21.8
	$10*A10+4*A1+2*A11+2*A4$					[289]
$C_{18}H_{22}N_4$	2,3-dimethyl-2,3-bis(phenylazo)butane					
342.3	21.09	0	61.6	76.8	21.09	26.3
	$4*A1+2*A4*B4+10*A10+2*A12+4*A42$					[258]
$C_{18}H_{22}O_2$	(dl) anisylidenecamphor					
371.5	26.36	0	70.95	67.9	26.36	25.2
	$2*A14+A15+4*A1+A114+A17+A16+A6+4*A10+2*A12+A32+A19+A17$					[273]
$C_{18}H_{22}O_2$	(d) anisylidenecamphor					
399.5	30.12	0	75.41	67.9	30.12	27.1
	$2*A14+A15+4*A1+A114+A17+A16+A6+4*A10+2*A12+A32+A19+A17$					[273]
$C_{18}H_{22}O_2$	di- α -cumyl peroxide					
312.4	28.14	0	90.08	90.1	28.14	28.2
	$4*A1+2*A4*B4+2*A11+10*A10+A33$					[216]
$C_{18}H_{23}FO_2$	4- <i>trans</i> -(4-fluorophenylethyl)cyclohexyl (E)-butenoate					
335.2	25	0	74.58	92.9	25	31.1
	$4*A10+A11+A12+2*A2+A14+3*A15+A16+A16+A38+A24+A1+A6+A6*B6$					[140]
$C_{18}H_{28}Si_4O_4$	1,1,3,3,5,5-hexamethyl-7,7-diphenylcyclotetrasiloxane					
305.0	42.73	0	140.12	78.4	42.73	23.9
	$6*A1+10*A10+2*A11+4*A112+4*A139+A14+5*A15$					[216]
$C_{18}H_{30}O$	2,4,6-tri- <i>tert</i> -butylphenol					
405.2	19.46	0	48.01	52.5	19.46	21.3
	$3*A11+2*A10+9*A1+3*A4+A31+A12$					[220]
$C_{18}H_{30}O_4$	<i>p</i> -diacetylbenzene diethyl ketal					
168.2	1.31	7.76				
326.2	23.5	72.05	79.8	117.6	24.81	38.4
	$4*A10+2*A11+2*A4*B4+6*A1+4*A2+4*A32$					[216]
$C_{18}H_{32}O_2$	1,10-cyclooctadecanedione					
359.2	11.84	32.96				
371.2	27.03	72.81	105.78	86.2	38.87	32.0
	$A14+15*A15+2*A114$					[114]
$C_{18}H_{32}O_4$	1,8-cyclotetradecanedione bis ethylene ketal					
457.2	30.67	0	67.08	84	30.67	38.4
	$3*A14+13*A15+2*A17+4*A112$					[114]
$C_{18}H_{34}O_2$	<i>trans</i> -9-octadecenoic acid (elaidic acid)					
317.6	61.55	0	193.8	172.1	61.55	54.7
	$A1+14*A2*B2+2*A6+A36$					[216]
$C_{18}H_{34}O_2$	<i>cis</i> -9-octadecenoic acid					
286.5	39.6	0	138.24	172.1	39.6	49.3
	$A1+14*A2*B2+2*A6+A36$					[216]
$C_{18}H_{34}O_2$	<i>cis</i> -6-octadecenoic acid					
303.7	47.5	0	156.43	172.1	47.5	52.3
	$A1+14*A2*B2+2*A6+A36$					[216]
$C_{18}H_{36}$	<i>n</i> -dodecylcyclohexane					
258.8	45.84	0	177.11	150.0	45.84	38.8
	$A14+A16+A1+11*A2*B2+3*A15$					[216]
$C_{18}H_{36}$	cyclooctadecane					
298.2	29.29	98.22				
346.2	9.87	28.52	126.74	88.9	39.16	30.8
	$15*A15+A14$					[110]
$C_{18}H_{36}$	1,1-dimethylcyclohexadecane					
216.2	1.26	5.81				
221.2	0.42	1.89				
290.2	14.23	49.02	56.72	82.1	15.9	23.8
	$A14+13*A15+2*A1+A17$					[112]
$C_{18}H_{36}N_2O_2^*$	N,N'-di- <i>n</i> -hexyladipamide					
432	40.79	0	94.56	168.7	40.79	72.9
	$14*A2*B2+2*A1+2*A60$					[216]
$C_{18}H_{36}O_2$	octadecanoic acid					
342.5	61.21	0	178.66	180.2	61.21	61.7
	$16*A2*B2+A1+A36$					[216]
$C_{18}H_{36}O_2$	ethyl hexadecanoate					
296.4	15.09	0	50.93	180.6	15.09	53.5
	$2*A1+A38+14*A2*B2+A2$					[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
$C_{18}H_{36}O_4$ 373.0	2,2,11,11-tetramethyl-1,3,10,12-tetraoxacyclooctadecane 35.1	0	94.1	94.9	35.1	35.4 [47]
$C_{18}H_{37}NO$ 336.1	$A14 + 15*A15 + 4*A112 + 2*A17 + 4*A1$ N-butyl tetradecanamide 45	0	133.89	170.0	45	57.1 [217]
$C_{18}H_{37}NO$ 377.2	$2*A1 + 3*A2 + A60 + 12*A2*B2$ octadecanamide 59.91	0	158.84	194.8	59.91	73.5 [217]
$C_{18}H_{37}NO_3$ 384.6 366.1 393.1	$16*A2*B2 + A1 + A61$ N-hexadecylglycine 4.5	11.7				
	5.6	15.3				
	56.5	143.73	170.73	175.5	66.6	69.0 [249]
$C_{18}H_{37}NO_3$ 383.1	$15*A2*B2 + A1 + A44 + A36*B36 + A2$ N-dodecyl-L-lucine 33.5	0	87.44	147.3	33.5	56.4 [249]
$C_{18}H_{37}NO_3$ 341.1 356.6	$3*A1 + 11*A2*B2 + A3 + A3*A3 + A36*B36 + A44 + A2$ N-dodecyl-DL-leucine 28.9	84.73				
	31	86.93	171.66	147.3	59.9	52.5 [249]
$C_{18}H_{38}$ 301.3	$3*A1 + 11*A2*B2 + A3 + A3*B3 + A36*B36 + A44 + A2$ octadecane 61.5	0	204.6	184.5	61.5	55.6 [216]
$C_{18}H_{38}O$ 334.2	$2*A1 + 16*A2*B2$ octadecanol 70.08	0	209.7	178.0	70.08	59.5 [220]
$C_{18}H_{48}Si_6$ 226.3 439.2	$17*A2*B2 + A1 + A30$ 1,2,3,4,5,6-hexamethyl-1,2,3,4,5,6-hexaethylcyclohexasilane 3.8	16.79				
	1.8	4.1	20.89	90.1	5.6	39.6 [175]
$C_{19}H_{13}F_3O$ 424.9	$A14 + 3*A15 + 6*A139 + 12*A1 + 6*A2$ 4-ethoxy-4'-trifluoromethyldiphenylacetylene 32.73	0	77.03	62.9	32.73	26.7 [195]
$C_{19}H_{14}F_2$ 343.7	$A1 + A2 + A11 + 3*A12 + 8*A10 + 4*A9 + 3*A25 + A4*B4 + A32$ 4-n-propyl-3',4'-difluorodiphenylacetylene 22.03	0	64.1	66.4	22.03	22.8 [195]
$C_{19}H_{15}Cl$ 376.8	$A1 + 2*A2 + A11 + 4*A12 + 7*A10 + 4*A9 + 2*A24$ triphenylchloromethane 27.9	0	74.04	70.3	27.9	26.5 [216]
$C_{19}H_{16}$ 365.3	$15*A10 + 3*A11 + A22 + A4*B4$ triphenylmethane 21.97	0	60.13	66.0	21.97	24.1 [216]
$C_{19}H_{16}O_2$ 395.2	$15*A10 + A3 + 3*A11$ 2-fluorenyl-2-methyl-1,3-cyclopentanedione 24.6	0	62.25	57.4	24.6	22.7 [259]
$C_{19}H_{17}F_3O$ 315.8	$2*A14 + 4*A15 + 2*A114 + A17 + A1 + A16 + 4*A19 + 8*A10$ 4-n-pentoxy-2',3',4'-trifluorodiphenylacetylene 33.1	0	104.81	94.8	33.1	29.9 [196]
$C_{19}H_{18}F_2$ 323.1	$6*A10 + 6*A12 + 3*A24 + A32 + 4*A2 + A1 + 2*A9$ 4-n-pentyl-3',4'-difluorodiphenylacetylene 22.1	0	68.4	86.2	22.1	27.9 [196]
$C_{19}H_{18}O_2$ 394.2	$7*A10 + A11 + 4*A12 + 2*A24 + 4*A2 + A1 + 2*A9$ 2-methyl-2-diphenylmethyl-1,3-cyclopentanedione 34.3	0	87.01	59.7	34.3	23.5 [259]
$C_{19}H_{19}F$ 337.4	$A14 + 2*A15 + 2*A114 + A17 + A1 + A3 + 2*A11 + 10*A10$ 4-n-pentyl-4'-fluorodiphenylacetylene 25.6	0	75.87	84.5	25.6	28.5 [196]
$C_{19}H_{19}FO$ 330.9	$8*A10 + A11 + 3*A12 + A24 + 4*A2 + A1 + 2*A9$ 4-n-pentoxy-4'-fluorodiphenylacetylene 27.2	0	82.2	91.3	27.2	30.2 [196]
$C_{19}H_{20}F_3N_3O_3$ 350	$8*A10 + 4*A12 + A24 + 4*A2 + A1 + 2*A9 + A32$ 2-[3-(trifluoromethyl)-phenyl]amino-3-pyridinecarboxylic acid β -morpholino ethyl ester 34.5	0	98.57	91.1	34.5	31.9 [216]
$C_{19}H_{20}O_2$ 352.2	$A14 + 3*A15 + A112 + A119 + 2*A2 + A38 + 7*A10 + 3*A12 + A41 + A44 + A11 + A4*B4 + 3*A25$ 3-methyl-3-diphenylmethyl-2,4-pentanedione 25.1	0	71.27	77.6	25.1	27.3

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$C_{19}H_{21}NO$	349.2	33.93	0	77.0	33.93	26.9
						[259]
$C_{19}H_{23}NO$	73.41	0.19	2.62			
	321.6	30.91	96.1	104.4	31.1	33.58
						[253]
$C_{19}H_{24}O$	337.7	31.38	0	63.0	31.4	21.3
						[216]
$C_{19}H_{26}O_2$	428	29.45	0	68.81	29.45	25.9
						[219]
$C_{19}H_{28}N_2$	326.2	29.01	0	88.95	29.1	33.7
						[26]
$C_{19}H_{30}O_2$	455.5	27.15	0	59.6	27.15	27.7
						[216]
$C_{19}H_{38}O$	328	68.65	0	209.3	68.65	62.0
						[21]
$C_{19}H_{38}O$	330	66.67	0	202.04	66.67	62.4
						[21]
$C_{19}H_{38}O_2$	338	9.76	28.87			
	341.2	57.62	168.87	195.93	67.38	64.7
						[216]
$C_{19}H_{38}O_2$	310.9	64.4	0	205.8	64.4	59.7
						[391]
$C_{19}H_{39}NO_3$	374.1	65.3	0	174.55	65.3	66.0
						[249]
$C_{19}H_{39}NO_3$	334.6	14.9	44.53			
	365.1	20.6	56.42	100.95	35.5	58.0
						[249]
$C_{19}H_{39}NO_3$	370.1	68.1	0	184	68.1	58.8
						[249]
$C_{19}H_{40}$	296.0	13.67	46.2			
	304	47.4	155.9	202.1	61.07	58.7
						[216]
$C_{20}F_{42}$	149.5	0.67	4.48			
	202.9	11.25	55.45			
	437.9	80.33	183.44	243.37	92.25	92.6
						[67]
$C_{20}H_{12}$	551.0	31.88	0	57.87	31.88	24.1
						[216, 217]
$C_{20}H_{12}$	426.2	2.51	5.89			
	454.4	16.57	36.46	42.35	19.08	19.8
						[215]
$C_{20}H_{12}$	390.2	8.49	21.77			
	454.2	17.32	38.13	59.9	25.81	19.8
						[215]
$C_{20}H_{14}$	527.2	30.29	0	57.46	30.29	31.7
						[216]
$C_{20}H_{14}$						

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
461.2	38.9	0	84.35	58.9	38.9	27.2
$C_{20}H_{14}O_4$	14*A10+6*A12 phenolphthalein	0				[216]
534	51.05	0	95.59	114.34	51.05	61.06
$C_{20}H_{15}F_3O$	A14+2*A15+A115+2*A19+A17+2*A31+12*A10 4-propoxy-4'-trifluoromethyldiphenylacetylene	0				[216]
315.9	18.81	0	59.54	70.0	18.81	22.1
$C_{20}H_{16}F_2$	A1+2*A2+A11+3*A12+8*A10+4*A9+3*A25+A4*B4+A32 4- <i>n</i> -butyl-3',4'-difluorodiphenylacetylene	0	71.39	73.6	24.33	25.1
340.8	24.33	0				[195]
$C_{20}H_{18}O_2$	A1+3*A2+A11+4*A12+7*A10+4*A9+2*A24 2-fluoroenyl-2-methyl-1,3-cyclohexanedione	0	79.65	61.1	35.7	27.4
448.2	35.7	0				[259]
$C_{20}H_{18}O_2Sn$	2*A14+5*A15+2*A114+A17+A1+A16+4*A19+8*A10 (acetyloxy)triphenylstannane	0	105.44	89.8	41.92	35.7
397.6	41.92	0				[221]
$C_{20}H_{19}F_3O$	15*A10+3*A12+A1+A38+A110 4- <i>n</i> -hexyloxy-2',3',4'-trifluorodiphenylacetylene	0	95.65	85.3	30.8	27.5
322	30.8	0				[196]
$C_{20}H_{20}F_2$	A1+5*A2+6*A12+6*A10+2*A9+2*A24+A32 4- <i>n</i> -hexyl-3',4'-difluorodiphenylacetylene	0	77.17	78.5	24.3	24.7
314.9	24.3	0				[196]
$C_{20}H_{20}F_2O$	A1+5*A2+A11+5*A12+6*A10+2*A9+2*A24 4- <i>n</i> -hexyloxy-3',4'-difluorodiphenylacetylene	0	102.29	85.3	33.1	27.6
323.6	33.1	0				[196]
$C_{20}H_{20}F_2O$	A1+5*A2+6*A12+6*A10+2*A9+2*A24+A32 4- <i>n</i> -hexyloxy-2',4'-difluorodiphenylacetylene	0	106.26	85.3	34.1	27.4
320.9	34.1	0				[196]
$C_{20}H_{20}O_2$	A1+5*A2+6*A12+6*A10+2*A9+2*A24+A32 2-ethyl-2-diphenylmethyl-1,3-cyclopentanedione	0	73.78	66.8	28.2	25.5
382.2	28.2	0				[259]
$C_{20}H_{20}O_3$	A14+2*A15+2*A114+A17+A1+A3+2*A11+10*A10+A2 4,4-dimethyl-1,8-diphenyl-2,3,5-trioxabicyclo[4.3.0]non-7-ene	0	59.86	45.9	22.1	16.9
369.2	22.1	0				[257]
$C_{20}H_{22}O_2$	10*A10+A11+A12+2*A14+3*A15+A19+A18+A162+A17+A112+A113+2*A1 3-ethyl-3-diphenylmethyl-2,4-pentanedione	0	89.39	84.8	34.7	32.9
388.2	34.7	0				[259]
$C_{20}H_{26}O_2$	3*A1+A4*B4+2*A35+A3+10*A10+2*A11+A2 19-nor-17 α -ethylnyltestosterone	0	82.67	55.1	39.6	26.4
479	39.6	0				[216]
$C_{20}H_{26}O_2$	4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114 +A30*B30+A1+A8+A9 2- <i>tert</i> -butyl-4-methoxymethyl-6- α -methylbenzylphenol	0	79.1	74.8	29.4	27.8
371.7	29.4	0				[101]
$C_{20}H_{26}O_3$	5*A1+A4+A2+A3+4*A11+A12+7*A10+A31+A32 testosterone formate	0	66.22	66.2	26.36	26.4
398	26.36	0				[219, 396]
398.2	18.12	0	45.5	66.2	18.1	26.4
$C_{20}H_{28}O_2$	4*A14+5*A15+2*A17+4*A16+2*A1+A37+A19+A18*B18+A114 1-[3,5-di- <i>tert</i> -butyl-4-hydroxyphenyl]-5-hexyn-1-one	0	73.47	74.9	25.14	25.6
342.2	25.14	0				[39]
$C_{20}H_{30}O_3Si_3$	6*A1+2*A4+2*A10+2*A11+2*A12+3*A2+A8+A9+A31+A35 1,1,3,3-tetraethyl-5,5-diphenylcyclotrisiloxane	0	65.84	97.9	18.37	27.3
279.1	18.37	0				[216]
$C_{20}H_{32}$	4*A1+4*A2+10*A10+2*A11+3*A112+3*A139+A14+3*A15 10,10,13,13-tetramethylcyclohexadeca-1,5-diyne	0	58.25	63.8	18.83	20.6
323.2	18.83	0				[113]
$C_{20}H_{36}O_2$	4*A1+A14+13*A15+2*A17+4*A20 1,10-cycloicosanedione	0	168.28	98.7	55.06	32.3
327.2	55.06	0				[114]
$C_{20}H_{36}O_4$	A14+17*A15+2*A112 1,9-cyclohexadecanedione bis ethylene ketal	0	104.24	91.4	42.13	36.9
404.2	42.13	0				[114]
$C_{20}H_{40}$	3*A14+15*A15+2*A17+4*A112 1,1,9,9-tetramethylcyclohexadecane	0	68.93	82.6	25.1	30.1
364.2	25.1	0				[112]
	4*A1+A14+13*A15+2*A17					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$C_{20}H_{40}$	1,1,4,4-tetramethylcyclohexadecane					
303.2	25.1	0	82.8	82.6	25.1	25.1
	4*A1 + A14 + 13*A15 + 2*A17					[112]
$C_{20}H_{40}$	1,1-dimethylcyclooctadecane					
283.2	23.85	0	84.21	89.5	23.85	25.3
	A14 + 15*A15 + 2*A1 + A17					[110]
$C_{20}H_{40}O_2$	eicosanoic acid					
348.2	69.2	0	198.7	198.9	69.2	69.3
	18*A2*B2 + A1 + A36					[216]
$C_{20}H_{40}O_4$	2,2,6,6,10,10,14,14-octamethyl-1,3,9,11-tetraoxacyclohexadecane					
406.9	24.69	0	60.67	88.7	24.69	36.1
	8*A1 + 2*A17 + 2*A17 + A14 + 13*A15 + 4*A112					[117]
$C_{20}H_{41}NO$	N-hexyl tetradecanamide					
310	8	25.81				
328	7	21.34				
334	35	104.79	151.94	195.2	50	65.2
	2*A1 + 17*A2*B2 + A60					[260]
$C_{20}H_{41}NO_3$	N-tetradecyl-L-leucine					
377.5	32.4	0	85.83	166.0	32.4	62.7
	3*A1 + 13*A2*B2 + A3 + A3*B3 + A2 + A44 + A36*B36					[249]
$C_{20}H_{41}NO_3$	N-tetradecyl-DL-leucine					
320.1	1.8	5.62				
349.6	54.8	156.75	162.37	166.0	56.6	58.0
	3*A1 + 13*A2*B2 + A3 + A3*B3 + A2 + A44 + A36*B36					[249]
$C_{20}H_{42}$	<i>n</i> -eicosane					
308.8	67.8	0	219.6	203.1	67.8	62.7
	2*A1 + 18*A2*B2					[216]
$C_{21}H_{16}$	1,2'-dinaphthylmethane					
369.6	30.54	0	82.64	61.8	30.54	22.8
	14*A10 + 2*A11 + A2 + 4*A12					[216]
$C_{21}H_{17}F_3O$	4- <i>n</i> -butoxy-4'-trifluoromethyldiphenyl diacetylene					
414.3	25.37	0	61.24	77.1	25.37	32.0
	A1 + 3*A2 + A11 + 3*A12 + 8*A10 + 4*A9 + 3*A25 + A4*B4 + A32					[195]
$C_{21}H_{18}F_2$	4- <i>n</i> -pentyl-3',4'-difluorodiphenyl diacetylene					
355.1	30.86	0	86.91	80.7	30.86	28.7
	A1 + 4*A2 + A11 + 4*A12 + 7*A10 + 4*A9 + 2*A24					[195]
$C_{21}H_{21}NO$	N,N-dimethyl-2,2-diphenylbenzeneacetamide					
402	25.43	0	63.26	83.5	25.43	33.6
	15*A10 + 3*A11 + A4*B4 + 2*A1 + A59					[221]
$C_{21}H_{24}O_2$	3-propyl-3-diphenylmethyl-2,4-pentanedione					
349.2	27.1	0	77.61	91.9	27.1	32.1
	3*A1 + A4*B4 + 2*A35 + A3 + 10*A10 + 2*A11 + 2*A2					[259]
$C_{21}H_{24}O_3Si_3$	<i>cis</i> -1,3,5-trimethyl-1,3,5-triphenylcyclotrisiloxane					
374.3	43.07	0	115.07	79.2	43.07	29.7
	3*A1 + 15*A10 + 3*A11 + 3*A112 + 3*A139 + A14 + 3*A15					[216,99]
$C_{21}H_{24}O_3Si_3$	<i>trans</i> -1,3,5-trimethyl-1,3,5-triphenylcyclotrisiloxane					
320.9	43.66	0	136.07	79.2	43.66	25.4
	3*A1 + 15*A10 + 3*A11 + 3*A112 + 3*A139 + A14 + 3*A15					[216,99]
$C_{21}H_{28}O_3$	testosterone acetate					
413	27.88	0	67.51	67.7	27.88	27.9
413.2	22.5	0	54.5	67.7	22.5	27.9
	4*A14 + 5*A15 + 2*A17 + 4*A16 + 3*A1 + A19 + A18*B18 + A114 + A38					[219, 396]
$C_{21}H_{28}O_5$	prednisolone					
513	38.86	0	75.75	78.2	38.86	40.1
	4*A14 + 5*A15 + 2*A17 + A17 + 4*A16 + 2*A1					[219]
	+ 3*A30*E30 + A19 + 2*A18*B18 + A18 + A114 + A35 + A2					
$C_{21}H_{28}O_5$	cortisone					
495	36.86	0	74.46	74.1	36.86	37.2
	4*A14 + 5*A15 + A17 + 2*A17 + 3*A16 + 2*A1 + 2*A30*E30					[219]
	+ A19 + A18*B18 + 2*A114 + A35 + A2					
$C_{21}H_{30}O_2$	progesterone					
404	26.99	0	66.8	64.6	26.99	26.1
	4*A14 + 5*A15 + 2*A17 + 4*A16 + 3*A1 + A19 + A18*B18 + A114 + A35					[219]
$C_{21}H_{30}O_3$	deoxycorticosterone					
414	27.98	0	67.59	69.4	27.98	28.9
	4*A14 + 5*A15 + 2*A17 + 4*A16 + 2*A1 + A30*C30					[219]
	+ A19 + A18*B18 + 2*A114 + A35 + A2					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$C_{21}H_{30}O_4$ 454	corticosterone 33.32	0	73.39	84.1	33.32	38.7
	$4 * A_{14} + 5 * A_{15} + 2 * A_{17} + 5 * A_{16} + 2 * A_1 + 2 * A_{30} * D_{30} + A_{19} + A_{18} * B_{18} + A_{114} + A_{35} + A_2$					[219]
$C_{21}H_{30}O_5$ 486	hydrocortisone 35.84	0	73.75	82.9	35.84	40.3
	$4 * A_{14} + 5 * A_{15} + 3 * A_{17} + 4 * A_{16} + 2 * A_1 + 3 * A_{30} * E_{30} + A_{19} + A_{18} * B_{18} + A_{114} + A_{35} + A_2$					[219]
$C_{21}H_{35}N_3N_2$ 362.7	N-palmitoyl-pyrazinamide 51.82	0	142.87	192.5	51.82	69.8
	$A_1 + 14 * A_2 * B_2 + 3 * A_{10} + A_{12} + 2 * A_{41} + A_{71}$					[261]
$C_{21}H_{42}O$ 336.7	11-heneicosanone 76.2	0	226.31	207.7	76.2	69.9
	$2 * A_1 + A_{35} + 18 * A_2 * B_2$					[262]
$C_{21}H_{42}O$ 333.9	2-heneicosanone 77.65	0	232.55	207.7	77.65	69.4
	$2 * A_1 + A_{35} + 18 * A_2 * B_2$					[263]
$C_{21}H_{43}NO_3$ 349.1 366.6	N-hexadecyl-L-valine 29.1 54.8	83.36 149.48	232.84	177.5	83.9	65.1
	$3 * A_1 + A_3 + A_3 * B_3 + 15 * A_2 * B_2 + A_{44} + A_{36} * B_{36}$					[249]
$C_{21}H_{43}NO_3$ 375.1	N-hexadecyl-DL-valine 80.5	0	214.61	177.5	80.5	66.6
	$3 * A_1 + A_3 + A_3 * B_3 + 15 * A_2 * B_2 + A_{44} + A_{36} * B_{36}$					[249]
$C_{21}H_{44}$ 305.7 313.7	<i>n</i> -heneicosane 15.48 47.7	50.65 152.06	202.71	212.4	63.18	66.6
	$19 * A_2 * B_2 + 2 * A_1$					[216]
$C_{22}H_{12}$ 554.2	1,12-benzoperylene 17.37	0	31.34	43.2	17.37	24.0
	$12 * A_{10} + 4 * A_{13} + 6 * A_{12}$					[215]
$C_{22}H_{12}$ 435.2	<i>o</i> -phenylenepyrene 21.51	0	49.41	36.0	21.51	15.7
	$A_{14} + 2 * A_{15} + 5 * A_{19} + 12 * A_{10} + 2 * A_{13} + 3 * A_{12}$					[264]
$C_{22}H_{14}$ 637.2	picene 35.19	0	55.22	44.0	35.19	28.0
	$14 * A_{10} + 8 * A_{12}$					[264]
$C_{22}H_{14}$ 553.5	1,2:3,4-dibenzanthracene 25.82	0	46.65	44.0	25.82	24.3
	$14 * A_{10} + 8 * A_{12}$					[215]
$C_{22}H_{14}$ 544.2	1,2:5,6-dibenzanthracene 31.16	0	57.26	44.0	31.16	23.9
	$14 * A_{10} + 8 * A_{12}$					[215]
$C_{22}H_{14}O_4$ 425.1	1,4-bis(phenylglyoxaloyl)benzene 32.3	0	75.98	92.2	32.3	39.2
	$14 * A_{10} + 4 * A_{12} + 4 * A_{35}$					[216]
$C_{22}H_{18}F_2O$ 370	4-(6-hexenyloxy)-3',4'-difluorodiphenyldiacetylene 37.45	0	101.22	92.5	37.45	34.2
	$A_5 + A_6 + 4 * A_2 + 5 * A_{12} + 7 * A_{10} + 4 * A_9 + 2 * A_{24} + A_{32}$					[195]
$C_{22}H_{18}F_2O$ 364.4	4-(<i>cis</i> -4-hexenyloxy)-3',4'-difluorodiphenyldiacetylene 35.32	0	96.93	90.9	35.32	33.1
	$A_1 + 2 * A_6 + 3 * A_2 + 5 * A_{12} + 7 * A_{10} + 4 * A_9 + 2 * A_{24} + A_{32}$					[195]
$C_{22}H_{18}F_2O$ 364.6	4-(<i>cis</i> -3-hexenyloxy)-3',4'-difluorodiphenyldiacetylene 30.97	0	84.94	91.0	30.97	33.1
	$A_1 + 2 * A_6 + 3 * A_2 + 5 * A_{12} + 7 * A_{10} + 4 * A_9 + 2 * A_{24} + A_{32}$					[195]
$C_{22}H_{19}Br_2NO_3$ 372.9	(<i>S</i>)- α -cyano-3-phenoxybenzyl (1 <i>R</i>)- <i>cis</i> -3-(2,2-dibromovinyl)-2,2-dimethylcyclopropanecarboxylate 40.71	0	109.18	96.6	40.71	36.0
	$A_{14} + A_{17} + 2 * A_{16} + 2 * A_1 + A_6 + A_7 + 2 * A_{21} + A_{38} + A_3 * B_3 + A_{56} + 2 * A_{12} + A_{11} + 9 * A_{10} + A_{32}$					[221]
$C_{22}H_{24}O_3$ 351.2	4-methyl-4-propyl-1,8-diphenyl-2,3,5-trioxabicyclo[4.3.0]non-7-ene 16.6	0	47.27	60.1	16.6	21.1
	$10 * A_{10} + A_{11} + A_{12} + 2 * A_{14} + 3 * A_{15} + A_{19} + A_{18} + A_{16} + 2 * A_{17} + A_{112} + A_{113} + 2 * A_1 + 2 * A_2$					[257]
$C_{22}H_{28}$ 414	1,1'-diphenyl-1,1'-bicyclopentyl 31.38	0	75.77	67.4	31.38	27.9
	$2 * A_{14} + 4 * A_{15} + 2 * A_{17} + 2 * A_{11} + 10 * A_{10}$					[289]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)
$C_{22}H_{28}N_2O_2$ 394	(4R*,5'R*,5'R*)-5,5-diphenyl-3,3',4,4'-tetramethyl-2,2'-bioxazolidine 31.9	0	80.96	82.2	31.9	32.4 [185]
$C_{22}H_{28}N_2O_2$ 368.8	2*A14+4*A15+6*A16+2*A119+10*A10+2*A11+4*A1+2*A112 (2R*,3R*,6R*,7R*)-2,6-diphenyl-3,4,7,8-tetramethyl- <i>cis</i> -perhydro-[3,2- <i>b</i>][1,4]-oxazino- [3,2- <i>b</i>][1,4]-oxazine 20.9	0	54.03	82.2	20.9	31.8 [185]
$C_{22}H_{28}N_2O_2$ 379.4	2*14+4*A15+6*A16+2*A119+10*A10+2*A11+4*A1+2*A112 (2R*,3S*,6R*,7S*)-2,6-diphenyl-3,4,7,8-tetramethyl- <i>cis</i> -perhydro- [1,4]-oxazino-[3,2- <i>b</i>][1,4]-oxazine 18.4	0	48.5	82.2	18.4	31.2 [185]
$C_{22}H_{28}O_3$ 480	2*A14+4*A15+6*A16+2*A119+10*A10+2*A11+4*A1+2*A112 19-nor-17 α -ethynyl-17 β -acetoxy-4-androsten-3-one 27.3	0	56.88	62.2	27.3	29.9 [216]
$C_{22}H_{29}FO_5$ 539	4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114+A38+2*A1+A8+A9 dexamethasone 42.02	0	77.97	78.8	42.02	42.5 [219]
$C_{22}H_{30}O_3$ 393 393.2	4*A14+5*A15+2*A17+2*A17+4*A16+3*A1+3*A30*F30+A19 +2*A18*B18+A18+A114+A35+A2+A27 testosterone propionate 25.64 22.13	0 0	65.24 56.3	74.8 74.8	25.64 22.1	29.4 29.4 [219, 396]
$C_{22}H_{40}O_4$ 378.2	4*A14+5*A15+2*A17+4*A16+3*A1+A19+A18*B18+A114+A38+A2 1,10-cyclooctadecanedione <i>bis</i> ethylene ketal 33.56	0	88.72	98.8	33.56	37.4 [114]
$C_{22}H_{44}$ 359.2	3*A14+17*A15+2*A17+4*A112 1,1,10,10-tetramethylcyclooctadecane 39.58	0	110.19	90.0	39.58	32.3 [110]
$C_{22}H_{44}N_2O_2$ 415	A14+15*A15+4*A1+2*A17 N,N'-di- <i>n</i> -hexylsebacamide 53.56	0	129.29	206.0	53.56	85.5 [216]
$C_{22}H_{44}O_2$ 288.4 299.7	18*A2*B2+2*A1+2*A60 butyl octadecanoate 2.22 37.48	7.7 125.05	132.75	220.1	39.7	66.0 [79]
$C_{22}H_{44}O_2$ 313.5 396.7	2*A1+A38+19*A2*B2 ethyl eicosanoate 15.58 7.78	49.68 19.62	69.3	220.1	23.36	87.3 [216]
$C_{22}H_{44}O_4$ 374	2*A1+A38+19*A2*B2 2,2,13,13-tetramethyl-1,3,10,12-tetraoxacyclodocosane 61.9	0	165.51	109.7	61.9	41.0 [47]
$C_{22}H_{45}Br$ 303.8 317.2	A14+19*A15+4*A112+2*A17+4*A1 1-bromodocosane 23.14 44.98	76.15 141.8	217.95	231.1	68.12	73.3 [265]
$C_{22}H_{45}NO$ 343.1	A1+21*A2*B2+A21 N-hexyl hexadecanamide 57	0	166.13	213.9	57	73.4 [217]
$C_{22}H_{45}NO_3$ 367.1	2*A1+19*A2*B2+A60 N-hexadecyl-L-leucine 46.1	0	125.58	186.8	46.1	68.6 [249]
$C_{22}H_{45}NO_3$ 333.1 355.1	3*A1+15*A2*B2+A3+A3*B3+A2*B2+A44+A36*B36 N-hexadecyl-DL-leucine 4.3 60.6	12.91 170.66	183.57	186.8	64.9	66.3 [249]
$C_{22}H_{46}$ 315.2 316.1	3*A1+15*A2*B2+A3+A3*B3+A2*B2+A44+A36*B36 <i>n</i> -docosane 29.51 47.84	93.62 151.36	245.0	221.8	77.3	70.3 [227]
$C_{23}H_{15}ClO_3$ 416.5	2*A1+20*A2*B2 2-[(4-chlorophenyl)phenylacetyl]-1H-indene-13(2H)-dione 34.54	0	82.94	79.6	34.54	33.2 [221]
$C_{23}H_{21}F_3O$ 394.8	A14+2*A15+2*A19+A16+13*A10+2*A114+A22*D22+A35+A12+ 2*A11+A3*B3 4- <i>n</i> -hexyloxy-4'-trifluoromethyldiphenyldiacetylene 33.98	0	86.07	91.0	33.98	35.9 [195]
$C_{23}H_{22}O_6$	A1+5*A2+A11+3*A12+8*A10+4*A9+3*A25+A4*B4+A32 [2R-(2a,6aa,12aa)]-1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)- [1]benzopyrano[3,4- <i>b</i>]furo[2,3- <i>h</i>][1]benzopyran-6(6aH)-one (Rotenone)					

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)	
437.9	35.64	0	81.39	90.3	35.64	39.6	
$C_{23}H_{30}O_6$	3*A14+6*A15+2*A19+4*A19+3*A112+3*A16+A114+4*A10+2*A12+3*A1+2*A32+A5+A7 prednisolone acetate						[221]
511	38.67	0	75.67	81.4	38.67	41.6	
$C_{23}H_{30}O_6$	4*A14+5*A15+3*A17+4*A16+3*A1+2*A30*E30+A19+2*A18*B18+A18+A114+A35+A2+A38 cortisone acetate						[219]
509	38.43	0	75.5	78.8	38.43	40.1	
$C_{23}H_{32}O_2$	4*A14+5*A15+3*A17+3*A16+3*A1+2*A30*E30+A19+2*A18*B18+2*A114+A35+A2+A38 3,3'-di- <i>tert</i> -butyl-5,5'-dimethyl-2,2-dihydroxydiphenylmethane						[219]
403.7	29.33	0	72.65	75.7	29.33	30.6	
$C_{23}H_{32}O_3$	8*A1+2*A4+6*A11+2*A12+A2+2*A31+4*A10 estra-1,3,5(10)-triene-3- α -17 β pentanoate						[101]
420.7	29.45	0	70	96.2	29.45	40.5	
$C_{23}H_{32}O_3$	3*A14+4*A15+2*A19+4*A16+A17+A38+A31+3*A10+A12+2*A1+3*A2 testosterone butyrate						[137]
382	24.75	0	64.8	81.9	24.75	31.3	
382.2	25.3	0	66.2	81.9	25.3	31.3	
$C_{23}H_{32}O_4$	4*A14+5*A15+2*A17+4*A16+3*A1+A19+A18*B18+A114+A38+2*A2 deoxycorticosterone acetate						[219, 396]
430	29.66	0	68.98	79.4	29.66	34.1	
$C_{23}H_{32}O_6$	4*A14+5*A15+2*A17+4*A16+3*A1+A38+A19+A18*B18+A114+A35+A2 hydrocortisone acetate						[219]
496	36.95	0	74.49	87.0	36.95	43.2	
$C_{23}H_{44}O_5$	4*A14+5*A15+3*A17+4*A16+3*A1+2*A30*E30+A19+A18*B18+A114+A35+A2+A38 1-aceto-3-stearin						[219]
319.9	41.69	0	130.31	222.5	41.69	71.2	
$C_{23}H_{46}O$	2*A1+16*A2*B2+A3*B3+2*A38+A30*B30+2*A2 12-tricosanone						[216]
342.2	78.03	0	228.04	226.4	78.03	77.5	
$C_{23}H_{46}O_2$	2*A1+A35+20*A2*B2 methyl docosanoate						[19]
325.0	82.3	0	251.7	228.9	82.3	74.6	
$C_{23}H_{48}$	2*A1+A38+20*A2*B2 <i>n</i> -tricosane						[391]
313.7	21.76	69.37				74.1	
320.7	53.97	168.33	237.69	231.1	75.73	74.1	
$C_{24}F_{50}$	2*A1+21*A2*B2 perfluorodocosane						[227]
202.7	3.89	19.19				116.8	
465.2	100.8	216.7	235.9	251.1	104.7	116.8	
$C_{24}H_{12}$	44*A26+24*A4*B4+6*A25 coronene						[67]
710.5	19.2	0	27.02	42.8	19.2	30.4	
$C_{24}H_{14}$	12*A10+6*A12+6*A13 1,2:4,5-dibenzopyrene						[215]
520.2	30.5	0	58.63	43.5	30.5	22.6	
$C_{24}H_{14}$	14*A10+8*A12+2*A13 3,4:9,10-dibenzopyrene						[215]
556.8	27.87	0	50.05	42.5	27.87	24.2	
$C_{24}H_{14}$	14*A10+8*A12+2*A13 1,2:3,4-dibenzopyrene						[215]
501.2	24.68	0	49.24	42.5	24.68	21.8	
$C_{24}H_{18}$	14*A10+8*A12+2*A13 1, 3, 5-triphenylbenzene						[215]
446	33.4	0	74.89	88.6	33.4	39.5	
$C_{24}H_{18}$	18*A10+6*A12 <i>p</i> -quaterphenyl						[132]
233.0	0.41	1.78				52.0	
587.2	37.8	64.37	66.15	88.6	38.2	52.0	
$C_{24}H_{28}O_2Si_3$	18*A10+6*A12 1,1,1,5,5,5-hexamethyl-3,3-diphenyltrisiloxane						[157,215]
270.5	22.75	0	84.12	88.6	22.75	24.0	
$C_{24}H_{31}FO_5$	6*A1+2*A32+3*A109+10*A10+2*A11 triamcinolone acetamide						[216]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpcc}}$ (calcd)	
566	45.29	0	80.02	78.6	45.29	44.5	
$\text{C}_{24}\text{H}_{31}\text{FO}_6$	5*A14+5*A15+5*A17+4*A16+4*A1+2*A30*F30 +A19+2*A18*B18+A18+A114+A35+A2+A28+2*A112 dexamethasone acetate						[219]
503	37.72	0	75	85.1	37.72	42.8	
$\text{C}_{24}\text{H}_{32}$	4*A14+5*A15+4*A17+4*A16+4*A1+2*A30*F30 +A19+2*A18*B18+A18+A114+A35+A2+A28+A38 1,1'-diphenyl-1,1'-bicyclohexyl						[219]
455	29.71	0	65.27	74.8	29.71	34.0	
$\text{C}_{24}\text{H}_{34}$	2*A14+6*A15+2*A17+2*A11+10*A10 1,1-diphenyldodecane						[289]
191	1.92	10.08					
281.4	38.83	137.98	148.11	127.5	40.75	35.9	
$\text{C}_{24}\text{H}_{34}\text{O}_3$	10*A10+10*A2+A1+2*A11+A3 testosterone valerate						[216]
380	24.57	0	64.66	89.1	24.57	33.8	
380.2	30.96	0	81.45	89.1	31.0	33.8	
$\text{C}_{24}\text{H}_{40}$	4*A14+5*A15+2*A17+4*A16+3*A1+A19+A18*B18+A114+A38+3*A2 1-cyclohexyl-1-phenyldodecane						[219, 396]
275.8	35.17	0	127.58	129.8	35.17	35.8	
$\text{C}_{24}\text{H}_{44}\text{O}_4$	A14+3*A15+5*A10+A3+10*A2+A16+A1+A11 1,11-cycloeoicosanedione-bis-ethylene ketal						[216]
362.2	43.72	0	120.71	106.2	43.72	38.5	
$\text{C}_{24}\text{H}_{46}$	3*A14+19*A15+4*A112+2*A17 2,11-dicyclohexyldodecane						[114]
300.6	43.93	0	146.15	119	43.93	35.77	
$\text{C}_{24}\text{H}_{46}$	2*A14+2*A1+2*A16+8*A2+6*A15+2*A3 1,1-dicyclohexyldodecane						[216]
300.6	44.35	0	147.54	132.1	44.35	39.7	
$\text{C}_{24}\text{H}_{48}$	2*A14+2*A16+A1+10*A2+6*A15+A3 cyclotetraeicosane						[216]
297	38	127.95					
322	10.8	33.54	161.49	111.1	48.8	35.8	
$\text{C}_{24}\text{H}_{48}\text{O}_2$	21*A15+A14 ethyl docosanoate						[181]
312.3	9.58	30.68					
321.0	19.16	59.69	90.37	236.6	28.74	75.9	
$\text{C}_{24}\text{H}_{50}$	2*A1+A38+20*A2*B2+A2 <i>n</i> -tetracosane						[216]
321.3	31.3	97.42					
324.1	54.89	169.37	266.79	240.4	86.19	77.9	
$\text{C}_{25}\text{H}_{31}\text{FO}_8$	22*A2*B2+2*A1 triamcinolone						[216]
543	42.56	0	78.39	86.6	42.56	47.0	
$\text{C}_{25}\text{H}_{34}\text{O}_3$	4*A14+5*A15+4*A17+4*A16+2*A1+4*A30*F30 +A19+2*A18*B18+A18+A114+A35+A2+A28 19-nor-17 α -ethynyl-17 β -(2,2-dimethylpropionyloxy-4-androsten-3-one)						[219]
500	37.8	0	75.6	74.5	37.8	37.3	
$\text{C}_{25}\text{H}_{40}\text{O}_2\text{Si}_2$	4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114 +A38+4*A1+A8+A9+A4*B4 norethindrone pentamethyldisiloxy ether						[216]
355	22.9	0	64.51	80.1	22.9	28.4	
$\text{C}_{25}\text{H}_{46}\text{O}_6$	4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114 +6*A1+A8+A9+2*A32+2*A109 1,2-diaceto-3-sterin						[216]
208.3	45.56	0	218.72	229.7	45.56	47.8	
$\text{C}_{25}\text{H}_{52}$	3*A1+2*A2+3*A38+A3*B3+16*A2*B2 <i>n</i> -pentacosane						[216]
320.2	26.07	81.42					
326.7	57.74	176.76	258.18	249.8	83.81	81.6	
$\text{C}_{25}\text{H}_{52}$	2*A1+23*A2*B2 5,5-bis(3,3-dimethylbutyl)-2,2,8,8-tetramethylnonane						[216]
472.7	48.53	0	102.67	93.8	48.53	44.4	
$\text{C}_{26}\text{H}_{14}$	4*(3*A1+A4+2*A2)+A4 1,12-phenyleneperylene						[266]
541.5	17.28	0	31.91	43.1	17.28	23.3	
$\text{C}_{26}\text{H}_{18}$	14*A10+8*A12+4*A13 9,9'-bifluorenyl						[215]
519.2	36.9	0	71.07	72.6	36.9	37.7	

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)	
$C_{26}H_{26}OSi_2$ 322.0	2*A14+4*A15+8*A19+2*A16+16*A10 1,3-dimethyl-1,1,3,3-tetraphenyldisiloxane	26.58	0	82.55	95.6	26.58	30.8
	20*A10+4*A11+2*A1+ A32*C32+2*A109 dimethyltetraphenylcyclotrisiloxane	28.2	0	78.1	89.1	28.2	32.2
$C_{26}H_{38}$ 493	A14+3*A15+3*A112+3*A139+2*A1+20*A10+4*A11 2,3-dimethyl-2,3-bis(4- <i>tert</i> -butylphenyl)butane	43.93	0	89.11	57.4	43.93	28.3
	4*A11+10*A1+4*A4+8*A10 11-phenyleicosane	64.77	0	220.08	187.3	64.77	55.1
$C_{26}H_{52}$ 269.9	2*A1+17*A2*B2+A3+5*A10+A11 11-cyclohexyleicosane	48.7	0	180.44	189.6	48.7	51.2
	A14+A16+2*A1+9*A2*B2+3*A15+A3+8*A2 1,1,4,4,10,10,13,13-octamethylcyclooctadecane	6.74	15.77	61.79	91.2	26.9	40.0
$C_{26}H_{52}O_2$ 317.7 327.4	A14+15*A15+8*A1+4*A17 ethyl tetracosanate	11.2	35.27				
	2*A1+22*A2*B2+A38+A2 N-decyl hexadecanamide	22.94	70.07	105.34	255.2	34.14	83.6
$C_{26}H_{53}NO$ 333 347	5 63	15.02	181.56	196.57	251.2	68	87.2
	2*A1+23*A2*B2+A60 <i>n</i> -hexacosane	59.5	180.6	289.3	259.1	95.3	85.3
$C_{26}H_{54}$ 326.5 329.5	32.2 59.5	98.7					
	2A1+24*A2*B2 19-nor-17 α -ethynyl-17 β -(benzoyloxy-4-androsten-3-one)	41.5	0	78.15	74.2	41.5	39.4
$C_{27}H_{30}O_3$ 531	4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114+A38+A1+ 5*A10+A12+A8+A9	21.6	0	63.53	97.8	21.6	33.3
	spiro[8.5.0(3,7)]-3,5-diphenyl-1,2,8-trioxo-10,12-tetramethyltetradec-5-ene	15	0	38.54	52.7	15	20.5
$C_{27}H_{32}O_3$ 389.2	3*A14+5*A15+4*A17+10*A10+A11+A12+4*A1+A19+A18+A16+A113+A112 19-nor-17 α -ethynyl-17 β -(heptanoyloxy-4-androsten-3-one)	21.6	0	63.53	97.8	21.6	33.3
	4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114 +A38+2*A1+5*A2+A8+A9	59.05	177.82	265.68	268.4	87.59	89.2
$C_{27}H_{46}O$ 304.8 420.2	cholesterol	2.5	8.2				
	4*A14+5*A15+5*A16+2*A17+5*A1+3*A2+2*A3+A30+A19+A18 <i>tris</i> N,N-diisobutylamino-1,3,5-triazine	27.41	65.22	73.42	73.7	29.91	31.0
$C_{27}H_{54}N_6$ 372.6	35.81	0	96.11	99.1	35.81	36.9	
	12*A1+6*A3+6*A2+3*A43+3*A12+3*A41 <i>n</i> -heptacosane	2.26	7.11				
$C_{27}H_{56}$ 318 325.4 332.1	26.28 59.05	80.75 177.82					
	2*A1+25*A2*B2 1,2,4,5,8,9-tribenzopyrene	28.8	0	47.37	43.4	28.8	26.4
$C_{28}H_{16}$ 608	16*A10+10*A12+2*A13 1,4-bis(diphenylphosphino)butane	45.3	0	111.6	105.4	45.3	42.8
	2*A72+20*A10+4*A12+4*A2 1,1,3,3-tetramethyl-5,5,7,7-tetraphenylcyclotetrasiloxane	0.24	1.3				
$C_{28}H_{28}O_2P_2$ 405.9	1.05 27.05	3.85 78.13	83.29	98.2	28.34	34.0	
	4*A1+20*A10+4*A11+4*A139+4*A112+A14+5*A15						

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)	
$C_{28}H_{32}O_4Si_4$	373.4	1,1,5',7'-tetramethyl-1',3',5,7-tetraphenylcyclotetrasiloxane 24.62	0	65.93	98.2	24.62	36.7
		$4*A1 + 20*A10 + 4*A11 + 4*A139 + 4*A112 + A14 + 5*A15$					[216]
$C_{28}H_{40}$	432	1,1'-diphenyl-1,1'-bicyclooctyl 35.98	0	83.26	89.6	35.98	38.7
		$2*A14 + 10*A15 + 2*A17 + 2*A11 + 10*A10$					[289]
$C_{28}H_{56}$	439.2	1,1,5,5,11,11,15,15-octamethylcycloicosane 47.7	0	108.6	98.6	47.7	43.3
		$A14 + 17*A15 + 8*A1 + 4*A17$					[107]
$C_{28}H_{56}O_2$	322.7	ethyl hexacosanate 13.22	40.98				
	322.7	27.05	83.81	124.79	273.9	40.27	88.4
		$2*A1 + A38 + 24*A2*B2 + A2$					[216]
$C_{28}H_{58}$	331.3	<i>n</i> -octacosane 35.44	106.98				
	334.5	64.64	193.28	300.26	277.8	100.08	92.9
		$26*A2*B2 + 2*A1$					[216]
$C_{29}H_{35}FO_{10}$	508	triamcinolone diacetate 38.31	0	75.42	98.7	38.31	50.1
		$4*A14 + 5*A15 + 4*A17 + 4*A16 + 6*A1 + A19$ $+ 2*A18*B18 + A18 + A114 + A35 + A2 + A28 + 4*A38$					[219]
$C_{29}H_{44}O_2$	447.7	3,3',5,5'-tetra- <i>tert</i> -butyldiphenylmethane-4,4'-diol 42.97	0	95.98	76.4	42.97	34.2
		$12*A1 + 4*A4 + 6*A11 + 2*A12 + A2 + 4*A10 + 2*A31$					[101]
$C_{29}H_{60}$	331.4	<i>n</i> -nonacosane 29.71	89.65				
	336.6	66.11	196.43	286.08	287.1	95.81	96.6
		$2*A1 + 27*A2*B2$					[216]
$C_{30}H_{46}$	400	3,4-diethyl-3,4-bis(4- <i>tert</i> -butylphenyl)hexane 29.71	0	74.27	85.9	29.71	34.4
		$10*A1 + 4*A4 + 4*A11 + 8*A10 + 4*A2$					[289]
$C_{30}H_{46}O_2S$	417.2	<i>bis</i> -[3,5-di- <i>tert</i> -butyl-4-hydroxybenzyl]sulfide 43.1	0	103.3	85.6	43.1	35.7
		$12*A1 + 4*A4 + 6*A11 + 2*A12 + 2*A2 + 2*A31 + A84 + 4*A10$					[101]
$C_{30}H_{60}O_4$	406.4	2,2,6,6,9,9,13,13,17,17,20,20-dodecamethyl-1,3,12,14-tetraoxacyclodocosane 57.3	0	141	112.1	57.3	45.5
		$A14 + 19*A15 + 4*A112 + 6*A17 + 12*A1$					[47]
$C_{30}H_{60}$	411.2	1,1,4,4,12,12,15,15-octamethylcyclodocosane 58.58	0	142.45	106.0	58.58	43.6
		$A14 + 19*A15 + 4*A17 + 8*A1$					[107]
$C_{30}H_{61}Br$	313.2	1-bromotricosane 23.85	76.15				
	339.6	79.5	234.09	310.24	305.7	103.34	103.8
		$A1 + 29*A2*B2 + A21$					[265]
$C_{30}H_{62}$	335.3	triacontane 37.49	111.82				
	338.7	68.83	203.24	315.06	296.4	106.32	100.4
		$2*A1 + 28*A2*B2$					[216]
$C_{31}H_{44}O_2$	400.7	3,3'- <i>bis</i> -(1-cyclohexylethyl)-5,5'-dimethyldiphenylmethane-2,2'-diol 29.29	0	73.09	101.8	29.29	40.8
		$6*A11 + 2*A12 + 4*A10 + 2*A31 + 4*A1 + 2*A3 + 2*A14$ $+ 6*A15 + 2*A16 + A2$					[101]
$C_{31}H_{64}$	282.3	11- <i>n</i> -decylheneicosane 71.13	0	251.96	288.3	71.13	81.4
		$3*A1 + 27*A2*B2 + A3$					[216]
$C_{32}H_{14}$	729	ovalene 8.08	11.08				
	770.1	17.4	22.59	33.68	41.4	25.48	32.2
		$14*A10 + 8*A12 + 10*A13$					[264]
$C_{32}H_{39}ClO_2$	413	norethindrone-6-(4-chlorophenyl)hexanoate 28.8	0	69.73	109.1	28.8	45.0
		$4*A14 + 5*A15 + 4*A16 + A19 + 2*A17 + A18*B18 + A114 +$ $A38 + A1 + 4*A10 + A11 + A12 + A8 + A9 + 5*A2 + A22*B22$					[216]
$C_{32}H_{64}O_2$	334.7	ethyl triacontanoate 16.2	48.4				
	341.5	36.07	105.65	154.04	311.2	52.27	106.3
		$2*A1 + A38 + 28*A2*B2 + A2$					[216]
$C_{32}H_{64}O_4$	342.5	2,2,6,6,10,10,14,14,18,18,22,22-dodecamethyl-1,3,13,15-tetraoxacyclotetracosane 39.7	0	115.9	119.5	39.7	40.9

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
$C_{32}H_{66}$	$A14 + 21*A15 + 4*A112 + 6*A17 + 12*A1$ dotriacontane					[47]
338.7	41.38	122.18				
343.5	76.57	222.93	345.11	315.1	117.94	108.2
$C_{33}H_{34}O_3$	$2*A1 + 30*A2*B2$ norethindrone-biphenyl-4-carboxylate					[216]
462	31.6	0	68.4	88.8	31.6	41.0
$C_{33}H_{40}O_3$	$4*A14 + 5*A15 + 4*A16 + A19 + 2*A17 + A18*B18 + A114 + A38 + A1 + 9*A10 + 3*A12 + A8 + A9$ norethindrone-4-cyclohexybenzoate					[216]
482	38.6	0	80.08	87.0	38.6	41.9
$C_{33}H_{48}O_3$	$4*A14 + 5*A15 + 4*A16 + A19 + 2*A17 + A18*B18 + A114 + A38$ norethindrone- <i>trans</i> -3-(4-butylcyclohexyl)propionate					[216]
374	22.5	0	60.16	112.9	22.5	42.2
$C_{33}H_{48}O_3^*$	$4*A14 + 5*A15 + 4*A16 + A19 + 2*A17 + A18*B18 + A114$ norethindrone- <i>trans</i> -4-hexylcyclohexylcarboxylate					[216]
398	22.6	0	56.78	112.9	22.6	44.9
$C_{33}H_{68}$	$4*A14 + 5*A15 + 4*A16 + A19 + 2*A17 + A18*B18 + A114 + A38$ triacontane					[216]
344	105.0	0	305.2	324.4	105.0	111.6
$C_{34}H_{54}$	$2*A1 + 31*A2*B2$ 4,5-dipropyl-4,5-bis(4- <i>tert</i> -butylphenyl)octane					[216]
419	40.58	0	96.86	114.4	40.58	47.9
C_3H_70	$4*A4 + 4*A11 + 10*A1 + 8*A2 + 8*A10$ tetracontane					[289]
341.5	29.3	85.8				
345.9	79.96	231.1	316.96	333.7	109.24	115.4
$C_{35}H_{72}$	$2*A1 + 32*A2*B2$ <i>n</i> -pentatriacontane					[217]
344.7	41.09	119.2				
347.2	86.4	248.85	368.04	343.1	127.49	119.1
$C_{36}H_{18}$	$2*A1 + 33*A2*B2$ decacyclene					[216]
666	25.4	0	38.14	49.4	25.4	32.9
$C_{36}H_{24}$	$3*A14 + 6*A15 + 15*A19 + 3*A12 + 18*A10$ 1,3,5-tri- α -naphthylbenzene					[264]
472	42.26	0	89.53	88.2	42.26	41.6
$C_{36}H_{46}O_4$	$24*A10 + 12*A12$ 4',4'-didecanoyloxydiphenyl diacetylene					[56]
308	44.9	145.78				
403	42.2	104.71	250.49	183.0	42.2	73.7
$C_{36}H_{74}$	$8*A10 + 4*A12 + 4*A9 + 2*A38 + 16*A2 + 2*A1$ hexatriacontane					[216]
345.4	9.92	28.71				
347.1	30.54	88.01				
349.2	88.83	254.41	371.13	352.4	129.29	123.04
$C_{38}H_{50}O_4$	$2*A1 + 34*A2*B2$ 4,4'-diundecanoyloxydiphenyl diacetylene					[216]
339	18.1	53.39				
358	7.59	21.14				
399	36.2	90.73	165.26	197.2	61.59	78.7
$C_{38}H_{62}$	$8*A10 + 4*A12 + 4*A9 + 2*A38 + 18*A2 + 2*A1$ 5,6-dibutyl-5,6-bis(4- <i>tert</i> -butylphenyl)decane					[216]
386	43.1	0	111.65	143.0	43.1	55.2
$C_{39}H_{74}O_6$	$4*A4 + 4*A11 + 10*A1 + 12*A2 + 8*A10$ glyceryl trilaurate					[289]
319.5	123.51	0	386.57	360.3	123.51	115.1
$C_{40}H_{54}O_4$	$3*A1 + 30*A2*B2 + 2*A2 + A3*B3 + 3*A38$ 4,4'-didodecanoyloxydiphenyl diacetylene					[216]
374	50.2	134.22				
401	44	109.73	243.95	255.4	94.2	102.4
$C_{40}H_{82}$	$8*A10 + 4*A12 + 4*A9 + 2*A38 + 20*A2*B2 + 2*A1$ tetracontane					[216]
345.4	14.02	40.58				
353.2	133.44	377.82	418.4	389.7	147.46	137.7
	$2*A1 + 38*A2*B2$					[268]

Table 5. Experimental and calculated total phase change enthalpy and entropy of database—Continued

$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$C_{42}H_{66}O_{12}$	benzene-hexa- <i>n</i> -hexanoate					
251.6	25.67	102.02				
291.5	12.27	42.11				
348.3	162.59	466.85				
368.7	33.5	90.85	701.82	277.8	234.03	102.5 [216]
$C_{45}H_{86}O_6$	6*A12+6*A38+6*A1+24*A2 glyceryl trimyristate					
330.2	152.2	0	460.92	416.3	152.2	137.5 [216]
	3*A1+36*A2*B2+2*A2+A3*B3+3*A38					
$C_{51}H_{98}O_6$	glyceryl tripalmitate					
338.9	179.37	0	529.27	472.3	179.37	160.1 [216]
	3*A1+42*A2*B2+2*A2+A3*B3+3*A38					
$C_{51}H_{100}ClN_5$	2,4- <i>bis</i> -N,N-didodecylamino-6-chloro-1,3,5-triazine					
307.5	34.25	0	111.4	441.0	34.25	135.6 [267]
	4*A1+44*A2*B2+2*A43+A22*F22+3*A12+A41					
$C_{51}H_{102}N_6$	tris N,N-dioctylamino-1,3,5-triazine					
312.7	74.25	0	237.45	440.9	74.25	137.9 [267]
	6*A1+42*A2*B2+3*A41+3*A43+3*A12					
$C_{57}H_{110}O_6$	glyceryl tristearate					
345.7	203.26	0	587.97	532.6	203.26	184.1 [216]
	3*A1+48*A2*B2+2*A2*B2+A3*B3+3*A38					
$C_{60}H_{78}Sn_2O$	hexakis(2-methyl-2-phenylpropyl)distanoxane					
417.7	71.81	0	171.92	165.8	71.81	69.3 [221]
	12*A1+6*A2+6*A4+30*A10+6*A11+2*A110+A32					
$C_{60}H_{122}$	hexacontane					
373.2	186.8	0	500.41	576.4	186.8	215.1 [268]
	2*A1+58*A2*B2					
$C_{63}H_{126}N_6$	tris N,N-didecylamino-1,3,5-triazine					
314.4	87.68	0	278.88	434.2	87.68	136.5 [267]
	6*A1+54*A2+3*A41+3*A43+3*A12					
$C_{75}H_{150}N_6$	tris N,N-didodecylamino-1,3,5-triazine					
320.3	119.19	0	372.12	519.8	119.19	166.5 [267]
	6*A1+66*A2+3*A41+3*A43+3*A12					
$C_{78}H_{108}$	2,3,6,7,10,11- <i>hexakis</i> (1-decynyl)triphenylene					
314.2	63	0	200.54	326.6	63	102.6 [216]
	6*7*A2+6*A1+6*2*A9+6*A10+12*A12					

^aUnits for $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ are $J \cdot mol^{-1} \cdot K^{-1}$ and $kJ \cdot mol^{-1}$, respectively; compounds with molecular formulas characterized with an asterisk (*) were not included in generating the statistics. As noted in the text, some of these compounds exhibit liquid crystal behavior, others display amphiphilic behavior, group values for some are not currently available or the error between experimental and calculated total phase change entropy exceeded 3 standard deviations.

TABLE 6. Experimental and calculated total phase change enthalpies and entropies of fusion of polymers^a

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
CF ₂ *	poly(tetrafluoroethylene)					
297	850	2.86				
605	4100	6.78	9.64	9.83	4.95	5.95
	A4*B4 + 2*A26					[389]
CH ₂ *	poly(ethylene)					
414.6	4.11	0	9.91	8.4	4.11	3.86
	A2*B2					[389]
CH ₂ O*	poly(oxymethylene)					
457.5	9.79	0	21.4	14.0	9.79	6.41
	A2*B2 + A32					[389]
C ₂ ClF ₃ *	poly(chlorotrifluoroethylene)					
493	5.02	0	10.2	15.8	5.02	7.8
	2*A4*B4 + 2*A26 + A27 + A22*F22					[389]
C ₃ HF ₃ *	poly(trifluoroethylene)					
495.2	5.44	0	11.0	12.4	5.44	6.3
	2*A4*B4 + 2*A26 + A27					[389]
C ₂ H ₂ F ₂ *	poly(vinylidene fluoride)					
483	6.70	0	13.9	16.9	6.7	8.18
	A2 + A4*B4 + 2*A26					[389]
C ₂ H ₂ O ₂ *	poly(glycolic acid)					
501	9.74	0	19.4	17.0	9.74	7.4
	A2*B2 + A38					[389]
C ₂ H ₃ Cl*	poly(vinylchloride)					
546	11.0	0	20.1	13.5	11.0	7.3
	A2 + A3*B3 + A22*C22					[389]
C ₂ H ₃ F*	poly(vinylfluoride)					
473	7.54	0	15.0	10.0	7.54	5.0
	A2 + A3*B3 + A27					[389]
C ₂ H ₄ O*	poly(oxyethylene)					
342	8.66	0	25.3	23.3	8.66	8.0
	2*A2*B2 + A32					[389]
C ₂ H ₄ O*	poly(vinyl alcohol)					
538	711	0	13.2	13.8	7.11	7.4
	A2 + A3*B3 + A30*C30					[389]
C ₂ H ₄ O ₂ *	poly(glycolide)					
501	11.75	0	23.5	17.0	11.75	8.5
	A3*B3 + A38					[216]
C ₃ H ₃ N*	poly(acrylonitrile)					
590	5.0	0	8.5	15.0	5.0	8.8
	A2 + A3*B3 + A56					[390]
C ₃ H ₄ O ₂ *	poly(β -propiolactone)					
366	10.9	0	29.8	26.3	10.9	9.6
	2*A2*B2 + A38					[389]
C ₃ H ₆ *	poly(propylene)					
460.7	8.70	0	18.9	8.3	8.7	3.8
	A1 + A2 + A3					[389]
C ₃ H ₆ O*	poly(propyleneoxide)					
348	8.40	0	24.1	19.6	8.4	6.8
	A1 + A2 + A3*B3 + A32					[389]
C ₃ H ₆ O*	poly(trimethyleneoxide)					
308	9.44	0	30.6	32.6	9.44	10.0
	3*A2*B2 + A32					[389]
C ₃ H ₆ O ₂ *	poly(oxymethylenoxyethylene)					
328	16.7	0	50.9	35.1	16.7	11.5
	2*A2*B2 + A2 + 2*A32					[389]
C ₄ H ₃ F ₃ O ₂ *	poly(vinyl trifluoroacetate)					
448	7.5	0	16.7	31.2	7.5	14.0
	A2 + A3*B3 + A4*B4 + A38 + 3*A25					[390]
C ₄ H ₄ O ₄ *	poly(ethylene oxalate)					

TABLE 6. Experimental and calculated total phase change enthalpies and entropies of fusion of polymers—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
450	23.0 2A2*B2+2*A38 poly(γ -butyrolactone)	0	51.1	34.0	23.0	15.3 [389]
C ₄ H ₄ O ₂ *	337.5	14.0 3*A2*B2+A38	0	41.5	14.0	12.0 [389]
C ₄ H ₅ Cl*	368	8.4 2*A2+A6+A7+A22*C22 <i>trans</i> -poly(chloroprene)	0	22.8	8.4	9.2 [390]
C ₄ H ₆ *	284.7	9.2 2*A2+2*A6 <i>cis</i> -poly(1,4-butadiene)	0	32.3	9.2	8.3 [389]
C ₄ H ₆ *	356	7.8 2*A2+2*A6 <i>trans</i> -poly(1,4-butadiene)	21.9			
	437	3.73	8.5	30.5	11.5	12.8 [389]
C ₄ H*	411	7.0 A1+2*A2+A3 poly(1-butene)	0	17.0	7.0	6.3 [389]
C ₄ H ₈ *	317	12.0 2A1+A2+A4 poly(isobutylene)	0	37.9	12.0	2.4 [389]
C ₄ H ₈ O*	330	14.4 4*A2*B2+A32 poly(oxytetramethylene)	0	43.6	14.4	13.8 [389]
C ₅ H ₈ *	301.2	4.35 A1+2*A2+A6+A7 <i>cis</i> -poly(isoprene)	0	14.4	4.35	8.0 [389]
C ₅ H ₈ *	347	12.8 A1+2*A2+A6+A7 <i>trans</i> -poly(isoprene)	0	36.9	12.8	9.2 [389]
C ₅ H ₈ Cl ₂ O*	463	32.0 4*A2+A4+2*A22*D22+A32 poly(2,2-bis(chloromethyl)trimethylene-3-oxide)	0	69.1	32.0	14.2 [389]
C ₅ H ₈ O ₂ *	450	9.5 2*A1+A2+A4*B4+A38 poly(methyl methacrylate)	0	21.1	9.5	12.2 [389]
C ₅ H ₈ O ₂ *	513	14.9 2*A1+A2+A4*B4+A38 poly(2,2-dimethylpropiolactone)	0	29.0	14.9	13.9 [389]
C ₅ H ₁₀ *	403.2	6.3 A1+2*A2*B2+A3 poly(1-pentene)	0	15.6	6.3	10.8 [389]
C ₅ H ₁₀ O ₂ *	296	14.3 A2+2*A2*B2+2*A32 poly(oxymethyleneoxytetramethylene)	0	48.3	14.3	15.9 [389]
C ₆ H ₄ O*	535	7.82 4*A10+2*A12+A32 poly(oxy-1,4-phenylene)	0	14.6	7.8	10.3 [389]
C ₆ H ₄ S*	593	8.65 4*A10+2*A12+A84 poly(thio-1,4-phenylene)	0	14.6	8.65	9.1 [389]
C ₆ H ₁₀ O ₂ *	342.2	17.9 4*A2*B2+A38 poly(ϵ -caprolactone)	0	52.3	17.9	18.5 [389]
C ₆ H ₁₀ O ₂ *	421	5.9 2*A1+2*A3*B3+A2+A38 poly(isopropyl acrylate)	0	14.0	5.9	12.8 [389]
C ₆ H ₁₁ NO*	533	26.0 5*A2*B2+A61 nylon-6 (poly(6-aminohexanoic acid))	0	48.8	26.0	25.6 [389]
C ₆ H ₁₂ *	523	10.0 2A1+2*A2+A3 poly(4-methyl-1-pentene)	0	19.0	10.0	8.7 [389]

TABLE 6. Experimental and calculated total phase change enthalpies and entropies of fusion of polymers—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
C ₈ H ₈ * 516.2	poly(styrene)					
	10.0	0	19.4	18.1	10.0	9.3
C ₈ H ₈ * 504 560 700	A2 + A3 + 5*A10 + A11					[389]
	poly(xylylene)					
	5.0	9.9				
	1.5	2.7				
C ₈ H ₈ O* 580	10.0	14.0	26.6	24.6	16.5	17.5
	4*A10 + 2*A11 + 2*A2					[389]
	poly(2,6-dimethyl-1,4-diphenylene oxide)					
C ₈ H ₁₂ O ₄ * 320 338	5.95	0	10.3	20.5	5.95	11.9
	2*A1 + 2*A10 + 2*A11 + 2*A12 + A32					[389]
	poly(ester-2,6 (poly(ethylene adipate)))					
C ₈ H ₁₆ O* 347	15.9	0	49.7		15.9	
	21.0	0	62.1	66.8	21.0	22.6
	4*A2*B2 + 2*A2 + 2*A38					[389]
C ₁₀ H ₈ O ₄ * 553	29.3	0	84.4	79.1	29.3	27.5
	8*A2*B2 + A32					[389]
	poly(ethylene terephthalate)					
C ₁₁ H ₂₀ O ₂ * 365	26.9	0	48.6	44.2	26.9	24.4
	2*A2 + 4*A10 + 2*A12 + 2*A38					[389]
	poly(undecanolactone)					
C ₁₁ H ₂₁ NO* 493	39.5	0	108.2	100.7	39.7	36.8
	10*A2*B2 + A38					[389]
	nylon-11 (poly(11-aminoundecanoic acid))					
C ₁₂ H ₁₂ O ₄ * 518	44.7	0	90.7	94.5	44.7	46.6
	10*A2*B2 + A61					[389]
	poly(tetramethylene terephthalate)					
C ₁₂ H ₂₀ O ₄ * 356.2	32.0	0	61.8	58.4	32.0	30.3
	4*A2 + 4*A10 + 2*A12 + 2*A38					[389]
	poly(ester-2,10 (poly(ethylene decanedioate)))					
C ₁₂ H ₂₂ N ₂ O ₂ * 574	31.9	0	89.6	104.0	31.9	37.0
	8*A2*B2 + 2*A2 + 2*A38					[389]
	nylon-6,6,α (poly(hexamethylene hexanediamide))					
C ₁₂ H ₂₃ NO* 500	57.8	0	100.6	96.0	57.8	55.1
	10*A2*B2 + A61					[389]
	poly(12-aminododecanoic acid)					
C ₁₃ H ₂₄ O ₂ * 368	48.4	0	96.8	103.8	48.4	51.9
	11*A2*B2 + A61					[389]
	poly(tridecanolactone)					
C ₁₄ H ₁₀ O ₄ * 610	50.6	0	137.5	119.3	50.6	43.9
	12*A2*B2 + A38					[389]
	poly(ethylene naphthalene-2,6-dicarboxylate)					
C ₁₄ H ₁₆ O ₄ * 434	25.0	0	41.0	44.0	25.0	26.8
	2*A2 + 6*A10 + 2*A12 + 2*A38					[389]
	poly(hexamethylene terephthalate)					
C ₁₅ H ₂₈ N ₂ O ₂ * 500	35.0	0	80.6	72.6	35.0	31.5
	6*A2 + 4*A10 + 2*A12 + 2*A38					[389]
	nylon-6,9 poly(hexamethylene nonanediamide)					
C ₁₅ H ₂₈ O ₂ * 370.5	69.0	0	138.0	123.9	69.0	62.0
	14*A2*B2 + 2*A61					[389]
	poly(pentadecanolactone)					
C ₁₆ H ₂₈ O ₄ * 343	63.4	0	171.1	139.7	63.4	51.1
	14*A2*B2 + A38					[389]
	poly(decamethylene adipate)					
C ₁₆ H ₃₀ N ₂ O ₂ * 506	42.7	0	124.4	145.6	42.7	49.9
	14*A2*B2 + 2*A38					[389]
	nylon-6,10 (poly(hexamethylene decanediamide))					
C ₁₈ H ₁₂ O* 753 770	71.7	0	141.6	133.2	71.7	67.4
	14*A2*B2 + 2*A61					[389]
	poly(oxy-2,6-diphenyl-1,4-diphenylene)					
	12.2	0	16.2	48.5	12.2	36.5
	87.	0	113.0	48.4	87.0	37.4

TABLE 6. Experimental and calculated total phase change enthalpies and entropies of fusion of polymers—Continued

T (K)		ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
$\text{C}_{18}\text{H}_{32}\text{O}_4^*$ 338	$12^*A10 + 6^*A12 + A32$	polyester-9,9 (poly(nonamethylene nonanedioate)) 43.2	0	127.8	164.2	43.2	[389, 390]
	$16^*A2^*B2 + 2^*A38$						55.5 [389]
$\text{C}_{18}\text{H}_{24}\text{O}_4^*$ 411	$16^*A2^*B2 + 2^*A38$	poly(decamethylene terephthalate) 46.1	0	112.1	123.0	46.1	50.6 [389]
	$10A2^*B2 + 4^*A10 + 2^*A38$						78.9 [389]
$\text{C}_{18}\text{H}_{32}\text{N}_2\text{O}_2^*$ 520	$16^*A2^*B2 + 2^*A61$	nylon-6,12 (poly(hexamethylene dodecanediamide)) 80.1	0	154.0	151.8	80.1	38.6 [389]
	$12^*A10 + 6^*A12 + 2^*A32 + A35$						37.4
$\text{C}_{19}\text{H}_{12}\text{O}_3^*$ 668.2	$12^*A10 + 6^*A12 + 2^*A32 + A35$	poly(oxy-1,4-phenylene-oxy-1,4-phenylene-carbonyl-1,4-phenylene) 37.4	0	56.0	57.8	37.4	38.6 [389]
	$18^*A2^*B2 + 2^*A38$						50.2
$\text{C}_{20}\text{H}_{36}\text{O}_4^*$ 353	$18^*A2^*B2 + 2^*A38$	poly(decamethylene-sebacate) 50.2	0	142.2	182.8	50.2	64.5 [389]

^aThese compounds were not included in generating the statistics.

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids^a

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
CBr ₂ Cl ₂	dibromodichloromethane					
	258.8	5.4	21.0			
	294.4	2.3	7.9	28.8	44.4	13.1
CHBr ₃	$A4 * B4 + 2 * A21 + 2 * A22 * D22$					
	281.5	11.1		39.4	42.7	12.0
CH ₂ O*	tribromomethane					
	281.4	12.68		45.1		12.7
CH ₂ F ₂	formic acid					
	136.4	4.4		32.0	39.9	5.4
CH ₂ I ₂	Group value not available					
	279.2	12.1		43.2	45.9	12.8
CH ₃ Br	diiodomethane					
	179.5	6.0		33.3	35.1	6.3
CH ₃ I	bromomethane					
	206.8	9.1		44.1	37.0	7.7
CH ₄ *	iodomethane					
	90.7	0.94		10.4		0.94
CH ₄ N ₂ O*	methane					
	408.1	12.9		31.7		12.9
	406.5	14.8		36.4		14.8
CH ₄ N ₂ S*	Group value not available					
	406	14.5		35.7		14.5
	452.2	12.6		27.8		12.6
CH ₆ BrN	thiourea					
	397.7	1.6	4.0			
	488.4	3.51	7.2			
COS*	methylammonium bromide					
	531.9	8.34	15.7	26.9		11.85
	134.3	4.73		35.2		4.73
CS ₂ *	Group value not available					
	161.1	4.39		27.2		4.39
CSe ₂ *	Group value not available					
	229.5	6.36		27.7		6.36
C ₂ Cl ₃ F ₃ *	Group value not available					
	287.5	4.11		14.3		4.11
C ₂ Cl ₄ F ₂ *	1,1,1-trichlorotrifluoroethane					
	314.2	4.0		12.7	51.7	16.2
C ₂ F ₄ O*	Forms plastic crystal					
	113.7	4.87		42.8		4.7
C ₂ F ₂ O ₂ *	1,1,1,2-tetrachlorodifluoroethane					
	260.7	13.4		51.4		13.4
C ₂ HF ₅	Group value not available					
	172.6	2.25		13.0	39.9	6.8

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
C_2H_2		$A4 * B4 + A3 * B3 + 3 * A25 + 2 * A26$ acetylene				[306]
142.7	2.54	17.8				
192.4	3.76	19.5	37.3	29.8	6.3	5.7
$\text{C}_2\text{H}_2\text{AsCl}_3$		$2 * A8$ <i>trans</i> - β -(chlorovinyl)dichloroarsine				[322]
270.7	17.1		63.2	50.1	17.1	13.6
$\text{C}_2\text{H}_3\text{N}_3\text{O}_3$		$A98 + 2 * A6 * B6 + 3 * A22 * D22$ 1,1,1-trinitroethane				[369]
311.7	4.6	14.77				
329.2	11.7	35.60	50.4	47.7	16.3	15.8
$\text{C}_2\text{H}_3\text{N}_3\text{O}_7$		$A1 + 3 * A50 + A4 * B4$ 2,2,2-trinitroethanol				[329, 352]
312.5	18.0	57.6				
344.9	2.7	7.9	65.5	59.5	20.7	20.5
$\text{C}_2\text{H}_6\text{Cd}^*$		$A2 + 3 * A50 + A30 * D30 + A4 * B4$ dimethylcadmium				[352]
254.4	1.52	5.98				
270.5	7.84	29.0	35.0	33.2	9.36	9.0
$\text{C}_2\text{H}_3\text{BF}_4\text{N}^*$		$2 * A1 + A114$ dimethylammonium tetrafluoroborate				[328]
283.5	7.5	26.5				
375	3.5	9.3	35.8		11.0	
$\text{C}_2\text{H}_8\text{BrN}^*$		Group value not available ethylammonium bromide				[216]
369.9	12.1	32.6				
439.5	8.5	19.4	52.0		20.6	
C_2N_2^*		Group value not available cyanogen				[216]
245.3	8.11		33.1		8.11	
$\text{C}_3\text{H}_4\text{N}_4\text{O}_6^*$		Group value not available 1,3,3-trinitroazetidine				[216]
375.5	30.3		80.7		30.3	
$\text{C}_3\text{H}_6\text{N}_2\text{O}_5$		2,2-dinitropropanol				[303, 332]
281.7	15.06	53.5				
366.7	2.85	7.8	61.2	53.7	17.9	19.7
$\text{C}_3\text{H}_6\text{N}_2\text{O}_7^*$		$A1 + A2 + A4 * B4 + 2 * A50 + A30 * C30$ 2,2-dinitro-1,3-propanediol				[352]
341.2	21.34		62.5	71.7	21.34	24.3
$\text{C}_3\text{H}_9\text{In}^*$		$2 * A2 + 2 * A50 + 2 * A30 * D30 + A4 * B4$ (Decomposes before melting) trimethylindium				[352]
358.7	14.3		39.9	33.5	14.3	12.0
$\text{C}_3\text{H}_9\text{Tl}^*$		$3 * A1 + A105$ trimethylthallium				[304]
311.2	16.74		53.8	53.8	16.7	16.7
$\text{C}_3\text{H}_{10}\text{BrN}^*$		$3 * A1 + A143$ propylammonium bromide				[370]
464.6	13.3		28.7		13.3	
$\text{C}_4\text{F}_8\text{S}^*$		Group value not available octafluorotetrahydrothiophene				[216]
146.0	10.88	74.5				
266.7	2.09	7.8	82.4	45.3	13.0	12.1
$\text{C}_4\text{H}_3\text{Cl}_3\text{OS}^*$		$A14 + 8 * A28 + 4 * A17 + 2 * A15 + A131$ methyl trichlorothioacrylate				[317]
286.25	20.4		71.2		20.4	
$\text{C}_4\text{H}_4\text{Se}^*$		Group value not available selenophene				[216]
122.7	0.3	2.5				
192.8	1.11	5.73				
240.2	4.58	19.1	27.3		6.0	
$\text{C}_4\text{H}_6\text{O}_6^*$		Group value not available D-tartaric acid				[216]
445.1	32.3		72.6	85.2	32.3	37.9
$\text{C}_4\text{H}_6\text{O}_2$		$2 * A3 * B3 + 2 * A30 * D30 + 2 * A36 * D36$ vinyl acetate				[392]
180.6	8.46		46.8	47.9	8.5	8.7

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)	
$\text{C}_4\text{H}_6\text{O}_3$	A1 + A5 + A6 + A38 <i>p</i> -dioxanone 16.14		53.5	48.8	16.1	14.7	
						[353]	
$\text{C}_4\text{H}_6\text{O}^*$	A14 + 3*A15 + A115 + A112 cyclobutanone 10.8		48.8	35.7	10.8	7.9	
						[338]	
$\text{C}_4\text{H}_{10}\text{Te}^*$	A14 + A15 + A114 diethyl telluride 7.62		47.2	47.2	7.6	7.7	
						[393]	
$\text{C}_4\text{H}_{11}\text{AsO}_2^*$	2*A1 + 2*A2 + A140 diethylarsinic acid 19.9		48.3	25.4	19.9	10.4	
						[299]	
C_5F_{10}	2*A1 + 2*A2 + A142 perfluorocyclopentane 5.0	41.9					
		12.6	54.5	42.8	8.0	12.1	
C_5F_{12}	A14 + 2*A15 + 10*A28 + 5*A17 perfluoro- <i>n</i> -pentane 6.8		46.0	63.4	6.8	9.3	
						[335]	
$\text{C}_5\text{H}_7\text{NS}^*$	6*A25 + 6*A26 + 5*A4*B4 2,4-dimethylthiazole 2.90		13.0	51.7	2.9	11.5	
						[61]	
$\text{C}_5\text{H}_8\text{N}_2\text{O}_2$	A14 + 2*A15 + 2*A19 + A18*B18 + 2A1 + A131 + A118 3-methyl-2,5-piperazinedione 30.62		56.3	52.8	30.6	28.7	
						[375]	
$\text{C}_5\text{H}_8\text{O}^*$	A14 + 3*A15 + 2*A124 + A16 + A1 cyclopentanone 11.4		51.3	39.4	11.4	8.7	
						[393]	
$\text{C}_5\text{H}_{10}\text{N}_2\text{O}_2$	A14 + 2*A15 + A114 N-acetylsarcosinamide 27.4	0	66.4	59.0	27.4	24.2	
						[354]	
$\text{C}_5\text{H}_{11}\text{Br}$	2*A1 + A2 + A59 + A61 3-bromopentane 8.40		50.2	57.1	8.4	9.6	
						[312]	
$\text{C}_5\text{H}_{12}\text{O}$	2*A1 + 2*A2 + A3*B3 + A21 2-pentanol 8.48		42.4	41.3	8.5	8.3	
						[361]	
$\text{C}_5\text{H}_{12}\text{O}$	2*A1 + 2*A2 + A3*B3 + A30 3-pentanol 9.08		44.47	41.3	9.1	8.4	
						[361]	
$\text{C}_6\text{H}_3\text{ClN}_2\text{O}_4$	2*A1 + 2*A2 + A3*B3 + A30 2,4-dinitrochlorobenzene 20.2		62.0	51.3	20.2	16.7	
						[334]	
$\text{C}_6\text{H}_3\text{ClN}_2\text{O}_4$	3*A10 + 3*A12 + 2*A50 + A22*C22 2,6-dinitrochlorobenzene 18.95		52.5	51.3	19.0	18.5	
						[334]	
$\text{C}_6\text{H}_5\text{ClO}_3\text{S}$	3*A10 + 3*A12 + 2*A50 + A22*C22 4-chlorobenzene sulfonic acid 10.6		31.8	31.8	10.6	10.6	
						[348]	
C_6H_6	4*A10 + 2*A12 + A22*B22 + A145 2,4-hexadiyne 1.00		8.48	24	1.00	2.8	
						[152]	
$\text{C}_6\text{H}_7\text{NO}_2$	2*A1 + 4*A9 ethyl- α -cyanoacrylate 12.86		52.9	56.7	12.9	13.8	
						[350]	
$\text{C}_6\text{H}_8\text{N}_2\text{O}_2\text{S}$	A1 + A2 + A5 + A7 + A38 + A56 <i>p</i> -aminobenzene sulfonamide 1.63	4.0					
		54.7	58.7	64.4	25.7	28.3	
		23.0	52.4	56.4	64.4	24.7	28.3
						[305,395]	
$\text{C}_6\text{H}_8\text{O}_4$	4*A10 + 2*A12 + A45 + A96 1,6-anhydro-2-deoxy- β -D-arabino-hexopyranose 12.55		38.9	56.9	12.6	18.4	
						[376]	
$\text{C}_6\text{H}_8\text{O}_6^*$	2*A14 + 2*A15 + 4*A16 + 2*A30*D30 + 2*A112 L-ascorbic acid						

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)	
466.15	37.04		79.5	84.2	79.5	39.2	
$\text{C}_6\text{H}_9\text{NO}$	A 14 + 2*A 15 + 4*A 30*E 30 + 2*A 19 + A 16 + A 3*B 3 + A 2 + A 115 N-vinylpyrrolidone						[392]
	286.2	15.28	53.4	40.4	15.3	11.6	
$\text{C}_6\text{H}_{10}\text{B}_2\text{N}_4^*$	A 14 + 2*A 15 + A 6*B 6 + A 5 + A 114 + A 119 pyrazabole						[368]
	354.3	11.83	33.4		11.8		
$\text{C}_6\text{H}_{10}\text{N}_2\text{O}_2$	Group value unavailable						[123]
	556.1	30.6	55.1	55.7	30.6	31.0	
$\text{C}_6\text{H}_{10}\text{N}_2\text{O}_2$	3,6-dimethyl-2,5-piperazinedione						
	418.2	22.0	52.7	36.3	22.0	15.2	
$\text{C}_6\text{H}_{10}\text{O}^*$	A 14 + 3*A 15 + 2*A 124 + 2*A 16 + 2*A 1 1,4-dimethyl-2,5-piperazinedione						[375]
	221	8.51	38.5				
$\text{C}_6\text{H}_{10}\text{O}_5$	A 14 + 3*A 15 + 2*A 125 + 2*A 1 cyclohexanone						[375]
	242.6	1.25	5.2	43.7	43.1	9.8	
$\text{C}_6\text{H}_{10}\text{O}_5$	A 14 + 3*A 15 + A 114 1,6-anhydro- β -D-glucopyranose						[393]
	385	24.9	64.8	59.4	24.9	22.9	
$\text{C}_6\text{H}_{10}\text{O}_5$	2*A 14 + 2*A 15 + 5*A 16 + 3*A 30*E 30 + 2*A 112 1,6-anhydro- β -D-glucopyranose						[376]
	404	24.5	60.6	59.4	24.5	24.0	
$\text{C}_6\text{H}_{10}\text{O}_5$	2*A 14 + 2*A 15 + 5*A 16 + 3*A 30*E 30 + 2*A 112 1,6-anhydro- β -D-galactopyranose						[376]
	401	22.8	56.9	59.4	22.8	23.8	
$\text{C}_6\text{H}_{10}\text{O}_5$	2*A 14 + 2*A 15 + 5*A 16 + 3*A 30*E 30 + 2*A 112 1,6-anhydro- β -D-altropyranose						[376]
	375	2.43	6.5				
$\text{C}_6\text{H}_{10}\text{O}_5$	388 18.0						46.4
			52.8	59.4	23.1	20.4	
$\text{C}_6\text{H}_{10}\text{O}_5$	2*A 14 + 2*A 15 + 5*A 16 + 3*A 30*E 30 + 2*A 112 1,6-anhydro- β -D-mannopyranose						[376]
	364	18.3	50.2	59.4	18.3	21.6	
$\text{C}_6\text{H}_{11}\text{Cl}$	2*A 14 + 2*A 15 + 5*A 16 + 3*A 30*E 30 + 2*A 112 1-chloro-1-methylcyclopentane						[376]
	164.2	1.3	7.8				
$\text{C}_6\text{H}_{11}\text{FO}_5$	178.8 5.7						31.9
	189.1	0.7	3.9	43.6	46.2	8.74	
$\text{C}_6\text{H}_{11}\text{FO}_5$	A 14 + A 15*2 + A 1 + A 4*B 4 + A 22 2-deoxy-2-fluoro-D-glucopyranose						[377]
	427.2	38.2	89.4	79.0	38.2	33.8	
$\text{C}_6\text{H}_{11}\text{FO}_5$	A 14 + 3*A 15 + A 2 + A 112 + 4*A 30*E 30 + 5*A 16 + A 28 3-deoxy-3-fluoro-D-glucopyranose						[336]
	378.2	18.3	48.4	79.0	18.3	29.9	
$\text{C}_6\text{H}_{11}\text{FO}_5$	A 14 + 3*A 15 + A 2 + A 112 + 4*A 30*E 30 + 5*A 16 + A 28 6-deoxy-6-fluoro-D-glucopyranose						[336]
	412.2	27.2	66.0	74.3	27.2	30.6	
$\text{C}_6\text{H}_{11}\text{NO}_2^*$	A 14 + 3*A 15 + A 2 + A 112 + 4*A 30*E 30 + 5*A 16 + A 27 5,5-dimethylperhydro-1,3-oxazine-2-one						[336]
	440.1	28.50	64.8	64.8	28.5	28.5	
C_6H_{12}	2*A 1 + A 14 + 3*A 15 + A 17 + A 125 4-methylpent-1-ene						[297]
	118.9	4.93	41.5	48.5	4.9	5.8	
$\text{C}_6\text{H}_{12}\text{O}_5$	2*A 1 + A 2 + A 3 + A 5 + A 6 1-deoxy-D-glucopyranose						[326]
	403.2	27.4	68.0	76.3	27.4	30.8	
$\text{C}_6\text{H}_{12}\text{O}_5$	A 14 + 3*A 15 + A 2 + A 112 + 4*A 30*E 30 + 4*A 16 2-deoxy-D-glucopyranose						[336]
	398.7	34.5	86.5	76.3	34.5	30.4	
$\text{C}_6\text{H}_{12}\text{O}_5$	A 14 + 3*A 15 + A 2 + A 112 + 4*A 30*E 30 + 4*A 16 3-deoxy-D-glucopyranose						[336]
	387.2	32.6	84.2	76.3	32.6	29.5	
$\text{C}_6\text{H}_{12}\text{O}_5$	A 14 + 3*A 15 + A 2 + A 112 + 4*A 30*E 30 + 4*A 16 6-deoxy-D-glucopyranose						[336]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
409.2	22.7		55.5	72.1	22.7	29.6
$\text{C}_6\text{H}_{12}\text{O}_6$	$A14+3*A15+A1+A112+4*A30*E30+5*A16$ α -D-glucopyranose (α -D-glucose)					[336]
423.2	34.3		81.1	90.3	34.3	39.2
$\text{C}_6\text{H}_{12}\text{O}_6$	$A14+3*A15+5*A30*F30+A2+5*A16+A112$ D-mannopyranose					[336]
391.2	24.7		63.1	90.3	24.7	35.3
$\text{C}_6\text{H}_{12}\text{Si}$	$A14+3*A15+5*A30*F30+A2+5*A16+A112$ 1-trimethylsilyl-1-propyne					[378]
204.5	10.96		53.6	37.7	11.0	7.7
$\text{C}_6\text{H}_{14}\text{O}_6$	$4*A1+A9+A109$ L-Iditol					[208,309]
352.8	30.90		87.6	108.0	30.9	38.1
$\text{C}_6\text{H}_{15}\text{AsO}_2^*$	$2*A2+4*A3*B3+6*A30*F30$ dipropylarsinic acid					[325]
408	22.1		54	39.6	16.2	22.1
$\text{C}_7\text{H}_5\text{F}_4\text{NO}_2$	$2*A1+4*A2+A142$ 1,1,3-trihydrotetrafluoropropyl α -cyanoacrylate					[381]
154.0	0.30	2.04				
287.4	19.95	69.4	71.5	71.9	20.3	20.7
$\text{C}_7\text{H}_5\text{N}_3\text{O}_6$	$A5+A7+A56+A38+A2+4*A26+A3*B3+A4*B4$ 2,4,6-trinitrotoluene					[337]
352.2	23.4		66.5	53.4	23.4	18.8
$\text{C}_7\text{H}_8\text{O}_2$	$A1+3*A50+3*A12+A11+2*A10$ 4-methoxyphenol					[217]
328.4	18.30		55.7	57.2	18.3	18.8
$\text{C}_7\text{H}_{10}\text{N}_2\text{O}_2$	$4*A10+2*A12+A1+A31+A32$ 1,3,5-trimethyluracil					[301]
428.7	16.1		37.6	38.5	16.1	16.5
$\text{C}_7\text{H}_{12}\text{N}_2\text{O}_2$	$A14+A15*3+2*A125+3*A1+A18*B18+A19$ N-acetyl-L-prolinamide					[379]
417.5	29.3		70.3	66.3	29.3	27.7
$\text{C}_7\text{H}_{12}\text{O}^*$	$A14+3*A15+A61+A16+A1+A146$ cycloheptanone					[380]
227	12.4	54.6				
232.6	0.43	1.8				
259.3	1.39	5.4	61.8	46.8	14.2	12.1
$\text{C}_7\text{H}_{14}\text{N}_2\text{O}_2$	$A14+3*A15+A114$ N-acetyl-L-valinamide					[393]
509	39.1		76.8	56.0	39.1	28.5
$\text{C}_7\text{H}_{14}\text{O}$	$3*A1+A3*B3+A3+A61+A60$ 2-heptanone					[380]
237.7	19.71		82.9	77.0	19.7	18.3
$\text{C}_7\text{H}_{14}\text{O}$	$2*A1+4*A2*B2+A35$ 3-heptanone					[214]
236.0	17.53		74.3	74.8	17.5	17.7
$\text{C}_7\text{H}_{14}\text{O}$	$2*A1+3*A2*B2+A2+A35$ 4-heptanone					[214]
240.2	16.16		67.3	68.2	16.2	16.4
$\text{C}_7\text{H}_{14}\text{O}_6$	$2*A1+4*A2+A35$ 1-methoxy- α -D-glucopyranoside					[214]
424.2	37.6		88.6	83.9	37.6	35.6
$\text{C}_7\text{H}_{14}\text{O}_6$	$A14+3*A15+A1+A2+A32+A112+4*A30*E30+5*A16$ 3-methoxy- α -D-glucopyranoside					[336]
425.6	41.3		97.0	83.9	41.3	35.7
$\text{C}_7\text{H}_{14}\text{O}_6$	$A14+3*A15+A1+A2+A32+A112+4*A30*E30+5*A16$ methyl α -D-mannopyranoside					[336]
455.2	44.7		98.2	83.9	44.7	38.2
$\text{C}_7\text{H}_{15}\text{Br}$	$A14+3*A15+A1+A2+A32+A112+4*A30*E30+5*A16$ 1-bromoheptane					[336]
214.4	21.76		101.5	90.9	21.8	19.5
$\text{C}_8\text{BrF}_{17}$	$A1+6*A2*B2+A21$ 1-bromoperfluorooctane					[333]
146.4	1.60	10.93				
278.9	12.13	43.49	54.4	103.0	13.7	28.7
	$8*A4*B4+3*A25+14*A26+A21$					[310]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$\text{C}_8\text{H}_5\text{Br}_3$	2,4,5-tribromostyrene					
340.3	25.10		73.8	59.9	25.1	20.4
	$2^*A10+4^*A12+A5+A6+3^*A21$					[295]
$\text{C}_8\text{H}_8\text{O}_3$	5,6-dioxycarbonyl[2.2.1]bicyclohept-2-ene					
323.6	0.90	2.78				
342.4	8.70	25.41				
388.4	3.60	9.27	37.5	43.2	13.2	16.8
	$3^*A14+A15+A116+4^*A16+2^*A18$					[359]
$\text{C}_8\text{H}_{10}\text{O}_4$	<i>trans, trans</i> -2,6-octadiene-1,8-dioic acid					
439.0	11.04	25.13				
541.0	27.77	51.32	76.5	65.2	38.8	36.3
	$2^*A6+2^*A36^*B36+2^*A2$					[46]
$\text{C}_8\text{H}_{10}\text{O}_4$	<i>trans, cis</i> -2,6-octadiene-1,8-dioic acid					
380.0	22.78		60.0	65.2	22.8	24.8
	$2^*A6+2^*A36^*B36+2^*A2$					[46]
$\text{C}_8\text{H}_{12}\text{B}_2\text{Cl}_6\text{O}_5^*$	1,3-diethyl-1,3-bis(trichloroacetoxy)-1,3-diboroxane					
327.2	24.22		74.0		24.2	
	Group value unavailable					[186]
$\text{C}_8\text{H}_{12}\text{N}_2\text{O}_2$	1,3-dimethyl-5-ethyluracil					
354.4	19.4		54.8	45.6	19.4	16.2
	$A14+3^*A15+2^*A125+3^*A1+A2+A18^*B18+A19$					[379]
$\text{C}_8\text{H}_{14}\text{O}^*$	cyclooctanone					
174	2.51	14.4				
226.8	13.8	60.8				
318.7	2.87	9.0	84.3	50.5	19.2	16.1
	$A14+5^*A15+A114$					[393]
$\text{C}_8\text{H}_{16}\text{B}_2\text{O}_5^*$	1,3-diacetoxy-1,3-diethyl-1,3-diboroxane					
377.2	21.60		57.3		21.6	
	Group value unavailable					[186]
$\text{C}_8\text{H}_{16}\text{N}_2\text{O}_2$	N-acetyl-L-isoleucine amide					
529.6	41.8		78.9	63.1	41.8	33.4
	$3^*A1+A2+A3+A3^*B3+A60+A61$					[354]
$\text{C}_8\text{H}_{16}\text{N}_2\text{O}_2$	N-acetyl-L-leucine amide					
382	0.3	0.8				
404	16.55	41.0	41.8	63.1	16.9	25.5
	$3^*A1+A2+A3+A3^*B3+A60+A61$					[380]
$\text{C}_8\text{H}_{16}\text{O}^*$	cyclooctanol					
261.3	2.12	8.11				
295.0	2.06	6.98	15.1	38.9	4.2	11.5
	$A14+5^*A15+A16+A30$					[365]
	Authors did not report enthalpic data for all transitions					
$\text{C}_8\text{H}_{16}\text{O}_4^*$	12-crown-4					
290.7	22.46		77.3	71.5	22.5	20.8
	$A14+9^*A15+4^*A112$					[398]
$\text{C}_8\text{H}_{17}\text{Br}$	1-bromooctane					
218.2	24.69		113.2	100.2	24.7	21.9
	$A1+7^*A2^*B2+A21$					[333]
$\text{C}_8\text{H}_{18}\text{O}_4$	1,2,7,8-tetrahydroxooctane					
352.2	36.7		104.2	112.0	36.7	39.4
	$4^*A30^*D30+6^*A2+2^*A3^*B3$					[346,347]
$\text{C}_8\text{H}_{18}\text{Zn}^*$	di- <i>tert</i> -butyl zinc					
300.0	45.30		151.0	70.8	45.3	21.2
	$6^*A1+2^*A4^*B4+A111$					[294]
$\text{C}_8\text{H}_{18}\text{AsO}_2^*$	dibutylarsinic acid					
412	29.5		71.5	67.0	29.5	27.6
	$2^*A1+6^*A2^*B2+A142$					[381]
$\text{C}_9\text{H}_8\text{O}_3$	<i>endo</i> -5-norbornene-2,3-dicarboxylic anhydride					
367.2	15.7	42.8				
437.2	3.71	8.49	51.3	44.2	19.4	19.3
	$3^*A14+A15+2^*A18+4^*A16+A117$					[318]
$\text{C}_9\text{H}_8\text{O}_3$	<i>exo</i> -5-norbornene-2,3-dicarboxylic anhydride					
416.2	21.77		52.3	44.2	21.8	18.4
	$3^*A14+A15+2^*A18+4^*A16+A117$					[318]
$\text{C}_9\text{H}_8\text{O}_4$	4-acetoxybenzoic acid					
467.2	26.35		56.4	56.1	26.4	26.4
	$A1+A38+A36^*B36+4^*A10+2^*A12$					[307]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (calcd)
C ₉ H ₁₀ O ₂	2,3-dimethylbenzoic acid		43.8	44.1	18.3	18.4
	417.6	18.30				
C ₉ H ₁₀ O ₂	2*A1 + 3*A10 + 2*A11 + A12 + A36		51.0	44.1	22.6	19.5
	442.9	22.60				
C ₉ H ₁₂ O	3,5-dimethylbenzoic acid		50.0	53.4	14.6	15.6
	292.8	14.64				
C ₉ H ₁₄ O	2,6-diisopropylphenol		47.0	47.1	14.1	14.1
	300.5	14.11				
C ₉ H ₁₄ N ₂ O ₂	4*A1 + 3*A10 + 2*A3 + A31 + 2*A11 + A12		74.2	52.7	26.3	18.7
	355.0	26.3				
C ₉ H ₁₄ N ₂ O ₂	bicyclo[3.3.1]nonan-9-one		63.0	39.7	22.4	14.1
	354.7	22.4				
C ₉ H ₁₅ N ₃ O ₃ *	2*A14 + 3*A15 + 2*A16 + A114		71.4	75.8	32.6	34.7
	450.6	5.60				
C ₉ H ₁₅ N ₃ O ₃ *	1,3-dimethyl-5-propyluracil		74.2	65.5	32.2	32.9
	457.8	27.0				
C ₉ H ₁₅ N ₃ O ₃ *	A14 + 3*A15 + 2*A125 + 3*A1 + 2*A2 + A18*B18 + A19		74.2	65.5	32.2	32.9
	434.1	32.2				
C ₉ H ₁₆ O*	N-acetyl-glycyl-L-prolinamide		64.9	54.2	16.3	16.2
	247	5.60				
C ₉ H ₁₉ Br	12.4		123.4	109.5	30.1	26.63
	298	1.6				
C ₁₀ H ₁₀ N ₄ O ₂ S	A14 + 2*A15 + A1 + A2 + A146 + A61 + A60 + A35 + A16		58	78.8	31.2	42.5
	538.7	31.2				
C ₁₀ H ₁₂	N-acetyl-L-prolyl-glycinamide		37.5	48.3	7.1	9.2
	189.8	7.11				
C ₁₀ H ₁₂	A14 + 2*A15 + A1 + A2 + A146 + A61 + A60 + A35 + A16		46.2	48.3	9.8	14.7
	216.1	8.04				
C ₁₀ H ₁₂ O ₂ *	cyclononane		46.2	48.3	9.8	14.7
	304.7	1.79				
C ₁₀ H ₁₂ O ₂ *	1-bromononane		4.08	61.4	1.4	20.5
	333.2	1.36				
C ₁₀ H ₁₂ O ₂	A1 + 8*A2*B2 + A21		75.5	53.6	25.2	17.9
	333.6	25.2				
C ₁₀ H ₁₂ O ₃ *	sulfadiazine		65.9	67.3	27.2	28.7
	394.2	7.95				
C ₁₀ H ₁₂ O ₃ *	7*A10 + 3*A12 + 2*A41 + A95 + A45		65.9	67.3	27.2	28.7
	419.7	16.74				
C ₁₀ H ₁₂ O ₄	3*A14 + A15 + 4*A18 + 4*A19		62.5	69.8	28.7	32.0
	426.7	2.51				
C ₁₀ H ₁₄ O	2-acetyl-3,5-dimethylphenol		46.6	54.8	11.6	13.6
	247.7	11.55				
C ₁₀ H ₁₅ F*	2*A12 + 2*A11 + 2*A10 + 3*A1 + A31 + A38		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	acetophenone ethylene glycol ketal		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	A14 + 2*A15 + 2*A112 + A17 + A1 + 5*A10 + A11		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	4-n-propoxybenzoic acid		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	4*A10 + 2*A12 + 2*A2 + A1 + A36*B36 + A32		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	Forms liquid crystal		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	2,5-diethoxy-1,4-benzoquinone		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	2*A1 + 2*A2 + A14 + 3*A15 + 2*A18 + 2*A19 + 2*A32 + 2*A114		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	L-carvone		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	2*A1 + A5 + A7 + A16 + A18*B18 + A19 + A14 + 3*A15 + A114		6.77	37.9	1.50	8.4
	221.6	1.50				
C ₁₀ H ₁₅ F*	1-fluoroadamantane		6.77	37.9	1.50	8.4
	221.6	1.50				

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (calcd)
$C_{10}H_{16}$	3*A14+A15+3*A16+A17+A27 <i>d</i> -limonene					[145]
199.2	11.38		57.1	57.7	11.4	11.5
$C_{10}H_{16}N_2O_2$	2*A1+A5+A7+A16+A18+A19+A14+3*A15 1,3-dimethyl-5-butyluracil					[213,293]
312.1	22.0		70.5	59.8	22.0	18.7
$C_{10}H_{16}O^*$	A14+A15*3+2*A125+3*A1+3*A2+A18*B18+A19 1-hydroxyadamantane					[379]
369.2	2.50	6.8		26.9	2.5	9.9
$C_{10}H_{16}O^*$	3*A14+A15+3*A16+A17+A30 2-hydroxyadamantane					[172]
325.2	0.30	0.92				
391.2	3.74	9.56	10.5	32.1	4.0	12.6
$C_{10}H_{18}O^*$	3*A14+A15+5*A16+A30 cyclodecanone					[172]
294.9	24.3		82.3	57.9	24.3	17.1
$C_{10}H_{22}O$	A14+7*A15+A114 1-decanol					[393]
280.1	37.66		134.5	103.0	37.7	28.9
$C_{10}H_{23}AsO_2^*$	A1+9*A2*B2+A30 dipentylarsinic					[321]
405	36.0		88.8	85.6	36.0	34.7
$C_{10}H_{30}Si_5O_5$	2*A1+8*A2*B2+A142 decamethylcyclopentasiloxane					[381]
226.2	20.37		90.1	67.8	20.4	15.3
$C_{11}H_8N_2$	10*A1+5*A112+5*A139+A14+7*A15 9H-pyrido[3,4- <i>b</i>]indole					[121]
471.5	25.50		54.0	56.5	25.5	26.6
$C_{11}H_{12}N_4O_2S$	A14+2*A15+2*A19+2*A19+7*A10+A121+A41 sulfamerazine					[323]
515.2	31.6		61.2	79.4	40.9	31.6
$C_{11}H_{12}N_4O_3S$	6*A10+3*A12+A11+A1+2*A41+A95+A45 4-amino-N-(6-methoxy-3-pyridazinyl)benzenesulfonamide (sulphamethoxypyridazine)					[382]
453.4	22.30		49.2	86.2	22.3	39.1
$C_{11}H_{12}N_2O^*$	6*A10+4*A12+A95+A45+2*A41+A1+A32 antipyrine					[194]
385.8	24.52		63.6	49.1	25.4	19.0
$C_{11}H_{13}N_3O_3S$	A14+2*A15+2*A1+A119+A125+5*A10+A12+A19+A18*B18 sulfisoxazole					[395]
468.2	29.2		62.5	83.1	29.2	38.9
$C_{11}H_{14}O_2^*$	4*A10+2*A12+A45+A95+A14+2*A15+3*A19+2*A1+A112+A118 2-acetyl-3,5-dimethylanisole					[382]
323.2	0.99		3.06	63.4	1.0	20.4
$C_{11}H_{14}O_3^*$	4*A1+2*A11+2*A12+2*A10+A32+A38 Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent 4- <i>n</i> -butoxybenzoic acid					[11]
420.7	18.83	44.8				
432.2	2.93	6.78	51.5	74.4	21.8	32.2
$C_{11}H_{16}O_2^*$	4*A10+2*A12+3*A2+A1+A36*B36+A32 Forms liquid crystal 1-adamantanecarboxylic acid					[178]
524.2	2.25		4.29	38.6	2.3	20.2
$C_{11}H_{20}O^*$	3*A14+A15+3*A16+A17+A36 Reported entropy is too small cycloundecanone					[149]
287.7	23.0		80.5	61.6	23.0	17.7
$C_{11}H_{23}Br$	A14+8*A15+A114 1-bromoundecane					[393]
263.3	33.47		127.1	128.1	33.5	33.7
$C_{12}HF_{25}^*$	A1+10*A2*B2+A21 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorododecane					[333]
344.5	23.00		66.76	137.9	23.00	47.5
$C_{12}H_8O_2S$	11*A4*B4+3*A25+22*A26+A3*B3 dibenzothiophene sulfone					[68]
507.8	23.72		46.7	40.4	23.7	20.5

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

<i>T</i> (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
C ₁₂ H ₁₀ N ₂	A 14+2*A 15+2*A 19+2*A 19+8*A 10+A 134					[327]
	1-methyl-9H-pyrido[3,4- <i>b</i>]indole 27.20		53.3	57.1	27.2	29.1
C ₁₂ H ₁₀ O ₂	A 1+A 14+2*A 15+2*A 9+2*A 19+6*A 10+A 11+A 121+A 41					[323]
	α -naphthyl acetate 20.21		63.3	54.6	20.2	17.4
C ₁₂ H ₁₀ O ₂	7*A 10+3*A 12+A 1+A 38					[118]
	β -naphthyl acetate 20.05		58.6	54.6	20.1	18.7
C ₁₂ H ₁₀ O ₂ S	7*A 10+3*A 12+A 1+A 38					[118]
	diphenyl sulfone 21.78		54.7	59.3	21.8	23.6
C ₁₂ H ₁₀ S	10*A 10+2*A 12+A 88					[327]
	diphenylsulfide 13.98		54.19	61.10	13.98	15.76
C ₁₂ H ₁₀ Te*	10*A 10+2*A 12+84					[207]
	diphenyl telluride 15.35		57.2	57.0	15.4	15.3
C ₁₂ H ₁₂ N ₂	10*A 10+2*A 12+A 140					[300]
	benzidine 19.10		47.7	72.0	19.1	28.8
C ₁₂ H ₁₄ N ₄ O ₂ S	4*A 12+8*A 10+2*A 45					[4]
	4-amino-N-[2,6-dimethyl-4-pyrimidinyl]benzene sulfonamide 45.11		87.5	58.6	45.1	30.2
C ₁₂ H ₁₄ N ₄ O ₂ S	2*A 1+5*A 10+3*A 12+2*A 11+2*A 41+A 95					[358]
	sulfisomidine 42.7		81.5	80.0	42.7	41.9
C ₁₂ H ₁₄ N ₄ O ₂ S	5*A 10+2*A 41+A 95+A 45+3*A 12+2*A 11+2*A 1					[382]
	sulfamethazine 31.1		66.0	80.0	31.1	37.7
C ₁₂ H ₁₆ O ₂ *	5*A 10+3*A 12+2*A 11+2*A 1+2*A 41+A 95+A 45					[382]
	4- <i>n</i> -pentylbenzoic acid					
	2.60	10.32				
	362.0	9.90	27.35			
C ₁₂ H ₁₆ O ₃ *	A 1+2*A 2+4*A 10+A 11+A 12+A 36					[177]
	Forms liquid crystal					
	4- <i>n</i> -pentoxybenzoic acid					
	21.8	54.7				
C ₁₂ H ₁₆ O ₄	4*A 10+2*A 12+4*A 2+A 1+A 36*B 36+A 32					[178]
	Forms liquid crystal					
	2,5-dipropoxy-1,4-benzoquinone					
	8.60	24.09				
C ₁₂ H ₁₆ O ₆	2*A 1+4*A 2+A 14+3*A 15+2*A 18*B 18+2*A 19+2*A 32+2*A 114					[342]
	α -phenoxy- α -D-glucopyranoside					
	39.0	90.9		95.8	39.0	41.1
	A 14+3*A 15+A 2+A 32+A 112+4*A 30*E 30+5*A 16+5*A 10+A 12					[384]
C ₁₂ H ₁₈ N ₂ O ₃ S*	3-(<i>p</i> -tolyl-4-sulfonyl)-1-butyl urea					
	25.6	63.3			25.6	
C ₁₂ H ₁₈ O	Group value not available					[358]
	2-(1'-cyclohexenyl)cyclohexanone					
C ₁₂ H ₁₈ O	17.26	61.9	59.0	17.3	16.5	[314]
	2*A 14+6*A 15+A 18+A 19+A 16+A 114					
C ₁₂ H ₁₈ O ₆	3,5-diisopropylphenol					
	12.13	37.2	53.4	12.1	17.4	[330]
C ₁₂ H ₁₈ O ₆	4*A 1+3*A 10+2*A 3+A 31+2*A 11+A 12					
	R,R,R-4,8,12-trimethyl-1,5,9-trioxacyclododeca-2,6,10-trione					
C ₁₂ H ₂₀ O	21.5	56.6	84.7	21.5	32.2	[206]
	3*A 1+A 14+9*A 15+3*A 115+3*A 16					
C ₁₂ H ₂₀ O	2-cyclohexylcyclohexanone					
	18.00	65.0	58.2	18.0	16.1	[314]
C ₁₂ H ₂₂ O	2*A 14+6*A 15+2*A 16+A 114					
	cyclododecanone					
C ₁₂ H ₂₂ O	16.85	50.2	65.3	16.9	21.9	
	16.6	50		16.6		
C ₁₂ H ₂₂ O	A 14+A 114+9*A 15					[298,393]
C ₁₂ H ₂₂ O	<i>trans</i> -2-cyclohexylcyclohexanol					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
325.8	14.52		44.6	46.6	14.5	15.2
$\text{C}_{12}\text{H}_{31}\text{AsO}_2^*$	2*A14+6*A15+3*A16+A30 dihexylarsinic acid					[313]
393	16.4	41.8				
405	24.35	60.1	101.9	104.2	40.7	42.2
$\text{C}_{12}\text{H}_{36}\text{O}_6\text{Si}_6$	2*A1+10*A2*B2+A142 dodecamethylcyclohexasiloxane					[381]
269.0	28.58		106.3	76.9	28.6	20.7
$\text{C}_{13}\text{H}_8\text{O}_2$	12*A1+6*A112+6*A139+A14+9*A15 S-(+)-4-isobutyl- α -methylphenyl acetic acid					[121]
325.5	18.70		57.5	57.5	18.7	18.7
$\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_2^*$	3*A1+A2+A3+A3*B3+4*A10+2*A11+A36 N-phenyl 4-nitrobenzaldehyde imine					[319]
347.15	24.56		70.7	64.0	24.6	22.2
$\text{C}_{13}\text{H}_{10}\text{O}_2^*$	9*A10+3*A12+A6*B6+A42+A50 (2-hydroxyphenyl)phenylmethanone					[397]
308.2	0.67		2.17		0.67	
$\text{C}_{13}\text{H}_{11}\text{N}^*$	No prediction made: Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent N-phenylbenzaldehyde imine					[11]
329.65	20.42		61.9	61.2	20.4	20.2
$\text{C}_{13}\text{H}_{12}\text{N}_2\text{O}^*$	10*A10+2*A12+A6*B6+A42 7-methoxy-1-methyl-9H-pyrido[3,4- <i>b</i>]indole					[397]
536.6	48.80		90.9	64.5	48.8	42.6
$\text{C}_{13}\text{H}_{17}\text{N}_3\text{O}^*$	2*A1+A14+2*A15+2*A19+2*A19+5*A10+A11+A121+A41+A32 aminopyrine					[323]
380	27.17		71.5	52.9	27.2	20.1
$\text{C}_{13}\text{H}_{18}\text{O}_2^*$	A14+2*A15+4*A1+A43+A119+A125+5*A10+A12+2*A19 4- <i>n</i> -hexylbenzoic acid					
371.0	17.40	46.90				
380.0	2.40	6.31	53.21	65.1	19.80	24.7
$\text{C}_{13}\text{H}_{18}\text{O}_2$	A1+2*A2+5*A10+A11+A12+A36 Forms liquid crystal benzaldehyde 2,2-dimethylpropylene glycol acetal					[177]
307.6	18.6		60.5	60.2	18.6	18.5
$\text{C}_{14}\text{H}_5\text{F}_{25}^*$	5*A10+A11+A14+3*A15+A17+A16+2*A1+2*A112 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorotetradecane					[385]
344.2	20.80		60.43	149.5	20.80	51.5
$\text{C}_{14}\text{H}_9\text{F}_{17}\text{O}_2^*$	12*A4*B4+3*A25+22*A26+A1+A2 Amphiphilic compound perfluorooctylethylene methacrylate					[68]
210	5.0	23.8				
253	9.0	35.6	59.4		14.0	
$\text{C}_{14}\text{H}_9\text{F}_{21}\text{O}^*$	Amphiphilic compound ω -perfluorodecyl-1-butanol					[16]
360	21.30		59.2		21.3	
$\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_2$	Amphiphilic compound 4-nitro-4'-methylbenzylidene aniline					[17]
402.0	27.30		67.9	64.6	27.3	25.9
$\text{C}_{14}\text{H}_{12}\text{O}_2^*$	A1+8*A10+A11+3*A12+A42+A6*B6+A50 (2-methoxyphenyl)phenylmethanone					[302]
350.2	0.68		1.94		0.7	
$\text{C}_{14}\text{H}_{14}\text{O}_3^*$	No prediction made: Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent Naproxen					[11]
428.5	31.5		73.5	58.6	31.5	25.1
$\text{C}_{14}\text{H}_{20}\text{O}_4$	2*A1+A3*B3+6*A10+A11+2*A12+A32+A36*B36 2,5-dibutoxy-1,4-benzoquinone					[394]
328.3	4.70	14.32				
364.5	2.30	6.31				
473.3	31.5	66.55	87.2	98.2	38.5	46.5
$\text{C}_{14}\text{H}_{22}$	2*A1+6*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114 1,4-di- <i>tert</i> -butylbenzene					[342]
341.5	22.48		65.8	46.4	22.5	15.9
$\text{C}_{14}\text{H}_{23}\text{NO}_2$	6*A1+4*A10+2*A11+2*A4 <i>n</i> -decyl- α -cyanoacrylate					[362]
294.5	41.80		142.0	133.3	41.8	39.3
	A1+9*A2*B2+A5+A7+A38+A56					[351]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
C ₁₄ H ₂₈	363.2	<i>trans</i> -1,4-di- <i>tert</i> -butylcyclohexane		47.2	17.2	18.6
		17.15				
C ₁₄ H ₂₈	293.2	6*A1 + A14 + 2*A15 + 2*A4 + 2*A16 <i>cis</i> -1,4-di- <i>tert</i> -butylcyclohexane		30.0	8.8	15.0
		8.79				
C ₁₄ H ₂₆ B ₂ N ₄ *	342.4 379.2	6*A1 + A14 + 2*A15 + 2*A4 + 2*A16 4,4,8,8-tetraethylpyrazabole		92.1	31.8	[41]
		28.61	83.61			
C ₁₄ H ₃₁ AsO ₂ *	299.0 389.0	Group value unavailable diheptylarsinic acid		153.0	122.8	50.4
		3.22	8.49			
C ₁₄ H ₄₂ O ₇ Si ₇	237.7	2*A1 + 12*A2*B2 + A142 tetradecamethylcycloheptasiloxane		87.8	86.0	20.9
		20.88				
C ₁₅ H ₁₁ NO ₂	443.2	14*A1 + 7*A112 + 7*A139 + A14 + 11*A15 1-(methylamino)-9,10-anthracenedione		65.0	49.1	21.8
		28.81				
C ₁₅ H ₁₂ CIN ₅ O ₄	500.2	A14 + 3*A15 + 2*A114 + 4*A19 + 7*A10 + A1 + A44 + A12 5-[4-chloro-2-nitrophenylazo]-1-ethyl-1,2-dihydro-6-hydroxy-4-methyl- 2-oxo-3-pyridinecarbonitrile		70.3	85.8	42.9
		35.16				
C ₁₅ H ₁₂ N ₂ O ₂	574.0	3*A10 + 3*A12 + A50 + A22*F22 + 2*A42 + A30*F30 + 2*A1 + A2 + A56 + A14 + 3*A15 + A125 + 4*A19 5,5-diphenylhydantoin		63.2	66.4	36.3
		36.29				
C ₁₅ H ₁₄ O ₂ *	405.2	A14 + 2*A15 + 2*A124 + A17 + 10*A10 + 2*A11 (2-hydroxy-4,6-dimethylphenyl)phenylmethanone		1.65	0.67	[395]
		0.67				
C ₁₅ H ₁₆ S ₂	329.0	No prediction made: Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent 2,2-bis(phenylthio)propane		74.2	75.4	24.4
		24.4				
C ₁₅ H ₂₀ N ₂ O ₄ S*	457.0	2*A1 + 10*A10 + 2*A12 + A4*B4 + 2*A84 4-acetyl-N-[(cyclohexylamino)carbonyl]benzene sulfonamide		89.9	41.1	[363]
		41.08				
C ₁₅ H ₂₁ NO ₂	308.2	Group value not available 1-methyl-4-phenylpiperidine-4-carboxylic acid ethyl ester (meperidine)		79.8	68.0	24.6
		24.60				
C ₁₆ H ₉ F ₂₅ *	147 314 349	2*A1 + 5*A10 + A11 + A38 + A14 + 3*A15 + A2 + A17 + A119 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafuorohexadecane		69.39	163.7	23.1
		0.70	4.76			
C ₁₆ H ₁₄ O ₃	367.4	1.40		4.46	41.1	[358]
		21.0	60.17			
C ₁₆ H ₁₆	404.0	3*A2 + A1 + 12*A4*B4 + 3*A25 + 22*A26 Amphiphillic compound (±)α-(3-benzoylphenyl)propionic acid		76.8	70.6	28.2
		28.23				
C ₁₆ H ₁₆	315.0 354.0	9*A10 + A11 + 2*A12 + A35 + A36*B36 + A1 + A3*B3 2,2-metacyclophane		53.0	51.3	21.4
		21.42				
C ₁₆ H ₁₆ *	323.2	A14 + 7*A15 + 4*A19 + 2*A18 + 6*A10 2,2-metaparacyclophane		39.2	46.0	13.7
		0.98	3.11			
C ₁₆ H ₁₆ O ₂ *	353.2	12.76		36.05	13.7	16.3
		0.21				
C ₁₆ H ₁₇ CIN ₄ O ₄ *	463.2	A14 + 8*A15 + 4*A19 + 3A18 + 5*A10 2,2-paracyclophane		0.65	40.7	0.2
		0.21				
C ₁₆ H ₁₆ O ₂ *	353.2	A14 + 9*A15 + 4*A19 + 4*A18 + 4*A10 (2-hydroxyphenyl)-2,4,6-trimethylphenylmethanone		1.39	0.49	[360]
		0.49				
C ₁₆ H ₁₇ CIN ₄ O ₄ *	463.2	No prediction made. Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent 2,2'-[[3-chloro-4-[(4-nitrophenyl)azo]phenyl]imino]bis-ethanol		64.3	29.8	[11]
		29.78				
		Group value not available				[13]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

<i>T</i> (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ (calcd)
$C_{16}H_{17}Cl_2N_5O_4^*$						
371.2	1-[[2-chloro-4-[(2-chloro-4-nitrophenyl)azo]-5-(methylamino)phenyl]amino]- 2-propanol N-oxide		82.5	82.5	30.6	30.6
	Group value not available					[315]
$C_{16}H_{17}F_{15}O^*$						
285.8	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7-pentadecafluoro-8-hexadecanone		119.7	147.5	34.2	42.2
	$7^*A4^*B4 + 3^*A25 + 12^*A26 + A1 + 7^*A2 + A35$					[23]
$C_{16}H_{20}O_3$						
387.6	Amphiphillic compound 3-benzoyl-1,2,2-trimethylcyclopentanecarboxylic acid		52.5	60.0	20.4	23.3
	$3^*A1 + A14 + 2^*A15 + 2^*A17 + A16 + 2^*A10 + A12 + A36^*B36 + A35$					[366]
$C_{16}H_{23}N^*$						
339.4	N-cyclohexyl(2,4,6-trimethyl)benzaldehyde imine		75.5	92.1	25.6	31.2
	$A14 + 3^*A15 + A16 + 3^*A1 + 2^*A10 + A6^*B6 + A42 + A12$					[397]
$C_{16}H_{24}O_4$						
333.7	2,5-dipentoxy-1,4-benzoquinone					
414.6		26.97				
		36.5	115.0	112.5	45.5	46.6
	$2^*A1 + 8^*A2 + A14 + 3^*A15 + 2^*A18^*B18 + 2^*A19 + 2^*A32 + 2^*A114$					[342]
$C_{16}H_{35}AsO_2^*$						
379	dioctylarsinic acid					
402		54.6				
		35.8	143.6	141.4	56.5	56.6
	$2^*A1 + 14^*A2^*B2 + A142$					[381]
$C_{17}H_{16}ClN_5O_3$						
428.2	3-[[4-[(2-chloro-4-nitrophenyl)azo]phenyl](2-hydroxyethyl)amino]propanenitrile		61.4	90.7	26.3	38.8
	$4^*A2 + 7^*A10 + 5^*A12 + A30^*F30 + A22^*F22 + A50 + A56 + 2^*A42 + A43$					[315]
$C_{17}H_{17}ClO_6^*$						
495.2	[(2S)- <i>trans</i> -7-chloro-,2',4,6-trimethoxy-6'-methylspiro[benzofuran- 2(3H),1'-(2)cyclohexene]-3,4'-dione		79.6	77.8	39.4	38.5
	$4^*A1 + A10 + 3^*A12 + 2^*A14 + 4^*A15 + A112 + 2^*A114 + 3^*A32 + A22^*F22 +$ $A17 + A18 + 3^*A19 + A16$					[357]
$C_{17}H_{17}Cl_2N_5O_4$						
471.2	N-[4-chloro-2-[(2-chloro-4-nitrophenyl)azo]-5-[(2-hydroxypropyl)amino]phenyl] acetamide		82.5	81.9	38.9	38.6
	$5^*A10 + 7^*A12 + 2^*A22^*F22 + 2^*A1 + A2 + A3^*B3 + A30^*F30 + A50 + 2^*A42$ $+ A60 + A44$					[315]
$C_{17}H_{19}NO_3$						
528.2	7,8-didehydro-4-5-epoxy-17-methylmorphinan-3,6-diol (morphine)		54.7	73.9	28.9	39.0
	$4^*A14 + 3^*A15 + 3^*A16 + A17 + A119 + A1 + 2^*A18 + A30^*D30 + 3^*A19 + 2^*A10 +$ $A12 + A112 + A31 + A114$					[296]
$C_{17}H_{19}NO_3$						
539.2	4,5-epoxy-3-hydroxy-17-methylmorphinan-6-one (hydromorphone)		66.0	54.8	35.6	29.5
	$2^*A10 + 4^*A14 + 3^*A15 + 3^*A19 + A31 + A112 + A1 + A119 + 3^*A16 + A12$ $+ A17 + A114$					[296]
$C_{17}H_{21}ClO_4$						
440.2	3-(3-chloro-4-methoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid		66.1	82.7	29.1	36.4
	$4^*A1 + A14 + 2^*A15 + 2^*A17 + A16 + 3^*A10 + 3^*A12 + A36^*D36 + A35$ $+ A32 + A22^*D22$					[366]
$C_{17}H_{21}F_{15}^*$						
220.0	1,1,1,2,3,3,4,4,5,5,6,6-dodecafluoro-2-(trifluoromethyl)hexadecane					
261.0		13.64				
		18.00	82.6	143.8	21.0	37.5
	$7^*A4^*B4 + 6^*A25 + A27 + 8^*A26 + A1 + 9^*A2$					[22]
$C_{17}H_{21}NO_6$						
426.9	Amphiphillic compound 3-(3-nitro-4-methoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid		75.8	84.2	32.4	35.9
	$4^*A1 + A14 + 2^*A15 + 2^*A17 + A16 + 3^*A10 + 3^*A12 + A36^*D36 + A35$ $+ A32 + A50$					[366]
$C_{17}H_{21}N_3O_2$						
384.2	2,2'-[[3-methyl-4-4(phenylazo)phenyl]imino]bis-ethanol		83.0	88.4	31.9	34.0
	$8^*A10 + 3^*A12 + A11 + 2^*A42 + A1 + 4^*A2 + 2^*A30^*E30 + A43$					[13]
$C_{17}H_{22}O_3$						
468.2	3-(4-methylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid		64.2	60.6	30.1	28.4
	$4^*A1 + A14 + 2^*A15 + 2^*A17 + A16 + 4^*A10 + A11 + A12 + A36^*B36 + A35$					[372]
$C_{17}H_{23}NO_3^*$						
422.0	3-[(hydroxyimino)phenylmethyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester		80.1	67.4	33.8	28.4
	$4^*A1 + A14 + 2^*A15 + A12 + 5^*A10 + 2^*A17 + A7 + A53 + A38 + A16$					[373]
$C_{17}H_{23}NO_4^*$						
498.6	3-(4-methoxy-3-aminobenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid		82.9	87.9	41.3	43.8
	$4^*A1 + A14 + 2^*A15 + 2^*A17 + A16 + 3^*A10 + 3^*A12 + A36^*D36 + A35 + A32 + A45$					[366]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{ipce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{ipce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{ipce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{ipce}}$ (calcd)
$\text{C}_{18}\text{HF}_{15}\text{Ge}^*$ 405.0	tris(pentafluorophenyl)germane 34.90			86.2	34.9	34.9
	18*A12+15*A24+A141					[308]
$\text{C}_{18}\text{H}_{11}\text{NO}_3$ 539.2	2-(3-hydroxy-2-quinoliny)-1H-indene-1,3(2H)-dione 30.89			57.3	30.9	43.3
	9*A10+4*A12+A14+2*A15+4*A19+A114+A30*D30+A41					[315]
$\text{C}_{18}\text{H}_{13}\text{F}_{25}^*$ 317.2 352.2	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorooctadecane 3.30 21.80					
	12*A4*B4+3*A25+22*A26+A1+5*A2 Amphiphillic compound		10.4 61.70	72.10	25.10	62.7
				177.9		[68]
$\text{C}_{18}\text{H}_{20}$ 274.5	6-(4-biphenyl)-1-hexene 15.10			55.0	15.1	25.5
	9*A10+2*A12+A11+4*A2+A5+A6					[97]
$\text{C}_{18}\text{H}_{20}$ 332.0 351.0 377.0	3,3-paracyclophane 7.36 0.46 11.76		22.17 1.31 31.19			
	A14+11*A15+4*A19+4*A18+4*A10			54.7	19.6	18.1
$\text{C}_{18}\text{H}_{20}\text{O}_2^*$ 380.2	(2-hydroxyl-4,6-dimethylphenyl)-2,4,6-trimethylphenylmethanone 0.84			2.21	0.84	
	Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					[11]
$\text{C}_{18}\text{H}_{21}\text{N}^*$ 339.6	N-benzyl-pivalophenone imine 27.86			82.05	27.9	28.6
	10*A10+A11+A12+3*A1+A4+A2+A6*B6+A42					[397]
$\text{C}_{18}\text{H}_{21}\text{NO}_3$ 430.3	7,8-didehydro-4,-5-epoxy-3-methoxy-17-ethylmorphanan-6-ol (codeine) 23.81			55.3	23.8	38.5
	2*A10+4*A14+3*A15+3*A19+A112+2*A1+A119+4*A16+A12+A17+A32+A30*D30+2*A18					[374]
$\text{C}_{18}\text{H}_{22}\text{O}_4$ 409.5 412.4	4,4'-di-(2-methoxyethoxy)biphenyl 17.53 22.67		42.81 54.97			
	2*A1+4*A2+8*A10+4*A12+4*A32			97.8	40.2	40.3
$\text{C}_{18}\text{H}_{24}\text{N}_2\text{O}_6^*$ 433.0	3-[(hydroxyimino)(4-methoxy-3-nitrophenyl)methyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester 31.99			73.9	32.0	33.6
	5*A1+A14+2*A15+3*A12+3*A10+2*A17+A16+A38+A32+A50+A7+A53					[373]
$\text{C}_{18}\text{H}_{24}\text{O}_3$ 387.6	3-(4-ethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid 22.54			58.2	22.5	26.3
	4*A1+A14+2*A15+2*A17+A16+4*A10+A2+A11+A12+A36*B36+A35					[366]
$\text{C}_{18}\text{H}_{24}\text{O}_3$ 460.6	3-(3,4-dimethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid 32.31			70.2	32.3	28.2
	5*A1+A14+2*A15+2*A17+A16+3*A10+2*A11+A12+A36*B36+A35					[366]
$\text{C}_{18}\text{H}_{24}\text{O}_3$ 386.8	3-(2,4-dimethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid 18.81			48.6	18.8	23.7
	5*A1+A14+2*A15+2*A17+A16+3*A10+2*A11+A12+A36*B36+A35					[366]
$\text{C}_{18}\text{H}_{24}\text{O}_4$ 394.6	3-(4-ethoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid 22.05			55.9	22.1	34.9
	4*A1+A14+2*A15+2*A17+A16+4*A10+A2+2*A12+A36*C36+A35+A32					[366]
$\text{C}_{18}\text{H}_{25}\text{NO}_3$ 445.0	3-[4-(dimethylamino)benzoyl]-1,2,2-trimethylcyclopentanecarboxylic acid 25.03			56.3	25.0	32.1
	5*A1+A14+2*A15+2*A17+A16+4*A10+2*A12+A36*C36+A35+A43					[366]
$\text{C}_{18}\text{H}_{25}\text{NO}_4^*$ 433.0	3-[(hydroxyimino)(4-methoxyphenyl)methyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester 36.99			85.4	37.0	32.4
	5*A1+A14+2*A15+2*A12+4*A10+2*A17+A16+A38+A32+A53+A7					[373]
$\text{C}_{18}\text{H}_{28}\text{O}_4$ 332.3 412.1	2,5-di- <i>n</i> -hexyloxy-1,4-benzoquinone 5.3 38.9		15.95 94.39			
	2*A1+10*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114			110.3	44.2	52.2
$\text{C}_{18}\text{H}_{32}\text{O}_2$ 303	linoelaidic acid 47.70			157.4	47.7	49.6
	A1+12*A2*B2+4*A6+A36					[331]
$\text{C}_{18}\text{H}_{32}\text{O}_2$	4-octadecynoic acid					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (calcd)
348	57.94		166.5	151.2	57.9	52.6
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 12 * A2 * B2 + 2 * A9 + A36 + 2 * A2$ 5-octadecynoic acid					[331]
325	54.41		167.4	149.0	54.4	48.4
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 11 * A2 * B2 + 2 * A9 + A36 + 3 * A2$ 6-octadecynoic acid					[331]
324	54.92		169.5	155.6	54.9	50.4
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A9 + A36$ 7-octadecynoic acid					[331]
322	53.61		166.5	155.6	53.6	50.1
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A9 + A36$ 8-octadecynoic acid					[331]
320	55.30		172.8	155.6	55.3	49.8
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A9 + A36$ 9-octadecynoic acid					[331]
319	54.87		172.0	155.6	54.9	49.6
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A9 + A36$ 10-octadecynoic acid					[331]
319	52.23		164.0	155.6	52.3	49.6
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A9 + A36$ 11-octadecynoic acid					[331]
320	55.97		174.9	155.6	56.0	49.8
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A9 + A36$ 12-octadecynoic acid					[331]
320	49.79		155.6	155.6	49.8	49.8
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A9 + A36$ 13-octadecynoic acid					[331]
322	55.51		172.4	155.6	55.5	50.1
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A9 + A36$ 14-octadecynoic acid					[331]
337	52.74		156.5	151.2	52.7	51.0
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 12 * A2 * B2 + 2 * A9 + A36 + 2 * A2$ 16-octadecynoic acid					[331]
347	60.10		173.2	155.6	60.1	54.0
$\text{C}_{18}\text{H}_{32}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A9 + A36$ 17-octadecynoic acid					[331]
340	54.20		159.4	157.7	54.2	52.9
$\text{C}_{18}\text{H}_{34}\text{B}_4\text{N}_4^*$	$15 * A2 * B2 + A9 + A36 + A8$ 4,4,8,8-tetrapropylpyrazobole		86.3		33.0	[331]
382.2	33.00					[123]
	Group value unavailable					[123]
$\text{C}_{18}\text{H}_{34}\text{O}_2$	<i>trans</i> -3-octadecenoic acid					[331]
334	57.15		171.1	169.6	57.2	56.7
$\text{C}_{18}\text{H}_{34}\text{O}_2$	$A1 + 13 * A2 * B2 + 2 * A6 + A36 + A2$ <i>trans</i> -4-octadecenoic acid					[331]
333	55.88		167.8	167.4	55.9	55.7
$\text{C}_{18}\text{H}_{34}\text{O}_2$	$A1 + 12 * A2 * B2 + 2 * A6 + A36 + 2 * A2$ <i>trans</i> -5-octadecenoic acid					[331]
319	45.11		141.3	165.2	45.1	52.7
$\text{C}_{18}\text{H}_{34}\text{O}_2$	$A1 + 11 * A2 * B2 + 2 * A6 + A36 + 3 * A2$ <i>trans</i> -6-octadecenoic acid					[331]
326	60.15		184.5	171.8	60.2	56.0
$\text{C}_{18}\text{H}_{34}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A6 + A36$ <i>trans</i> -10-octadecenoic acid					[331]
326	58.52		179.5	171.8	58.5	56.0
$\text{C}_{18}\text{H}_{34}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A6 + A36$ <i>trans</i> -11-octadecenoic acid					[331]
317	58.49		184.5	171.8	58.5	54.5
$\text{C}_{18}\text{H}_{34}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A6 + A36$ <i>trans</i> -12-octadecenoic acid					[331]
325	56.71		174.5	171.8	56.7	55.8
$\text{C}_{18}\text{H}_{34}\text{O}_2$	$A1 + 14 * A2 * B2 + 2 * A6 + A36$ <i>trans</i> -13-octadecenoic acid					[331]
318	55.62		174.9	165.2	55.6	52.5
$\text{C}_{18}\text{H}_{34}\text{O}_2$	$A1 + 11 * A2 * B2 + 2 * A6 + A36 + 3 * A2$					[331]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
$\text{C}_{18}\text{H}_{34}\text{O}_2$	<i>trans</i> -14-octadecenoic acid					
327	57.06		174.5	167.4	57.1	54.7
	$A1 + 12*A2*B2 + 2*A6 + A36 + 2*A2$					[331]
$\text{C}_{18}\text{H}_{34}\text{O}_2$	<i>trans</i> -15-octadecenoic acid					
331	58.98		178.2	169.6	59.0	56.1
	$A1 + 13*A2*B2 + 2*A6 + A36 + A2$					[331]
$\text{C}_{18}\text{H}_{36}$	<i>cis, cis</i> -1,3,5- <i>tri-tert</i> -butylcyclohexane					
393.2	26.78		68.1	54.4	26.8	21.4
	$9*A1 + A14 + 3*A15 + 3*A4 + 3*A16$					[41]
$\text{C}_{18}\text{H}_{36}$	<i>cis, trans</i> -1,3,5- <i>tri-tert</i> -butylcyclohexane					
338.2	17.99		53.2	54.4	18.0	18.4
	$9*A1 + A14 + 3*A15 + 3*A4 + 3*A16$					[41]
$\text{C}_{18}\text{H}_{38}\text{O}_2$	2-(hexadecyloxy)ethanol					
311.7	14.94	47.93				
318.5	37.32	117.2	165.1	193.7	52.3	61.7
	$A1 + 15*A2*B2 + A32 + A30*B30 + 2A2$					[88]
$\text{C}_{18}\text{H}_{38}\text{O}_9$	1, ω -dimethoxyocta(oxyethylene)					
276.2	60.1		217.6	226.4	60.1	62.5
	$2*A1 + 16*A2*B2 + 9*A32$					[386]
$\text{C}_{18}\text{H}_{39}\text{AsO}_2$	di- <i>n</i> -nonylarsinic acid					
383	24.3	63.5				
399	38.1	95.5	159	160	62.4	63.8
	$2*A1 + 16*A2*B2 + A142$					[381]
$\text{C}_{18}\text{H}_{54}\text{O}_9\text{Si}_9$	octadecamethylcyclononasiloxane					
246.2	25.64		104.1	104.2	25.6	25.7
	$18*A12 + 9*A139 + 9*A112 + A14 + 15*A15$					[121]
$\text{C}_{19}\text{H}_{21}\text{F}_{19}^*$	1,1,1,2,3,3,4,4,5,5,6,6,7,7,8,8-hexadecafluoro-2-(trifluoromethyl)octadecane					
274.0	1.00	3.65				
298.0	25.00	83.89	87.54	370.2	26.00	110.3
	$9*A4*B4 + 6*A25 + A27 + 12*A26 + A1 + 9*A2$					[22]
$\text{C}_{19}\text{H}_{15}\text{N}^*$	Amphiphillic compound N-phenyl benzophenone imine					
392.3	29.14		74.3	76.0	29.14	29.8
	$15*A10 + 3*A12 + A7 + A42$					[397]
$\text{C}_{19}\text{H}_{24}\text{O}_3^*$	3-[(2,3-dihydro-1H-inden-5-yl)carbonyl]-1,2,2-trimethylcyclopentanecarboxylic acid					
404.3	22.50		55.7	61.4	22.5	24.8
	$3*A1 + 2*A14 + 4*A15 + 2*A17 + A16 + 2*A19 + 3*A10 + A12 + A36*B36 + A35$					[366]
$\text{C}_{19}\text{H}_{26}\text{O}_4$	3-(4-methoxy-2,6-dimethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
416.7	28.31		67.9	82.6	28.3	34.4
	$6*A1 + A14 + 2*A15 + 2*A17 + A16 + 2*A10 + 2*A12 + 2*A11 + A36*C36 + A35 + A32$					[366]
$\text{C}_{19}\text{H}_{26}\text{O}_6$	1,2,2-trimethyl-3-(2,4,6-trimethoxybenzoyl)cyclopentanecarboxylic acid					
432.2	29.68		68.7	96.2	29.7	41.6
	$6*A1 + A14 + 2*A15 + 2*A17 + A16 + 2*A10 + 4*A12 + A36*E36$					[366]
	$+ A35 + 3*A32$					
$\text{C}_{19}\text{H}_{27}\text{NO}_3^*$	2-[(3,4-dimethylphenyl)(hydroxyimino)methyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
426.0	39.14		91.9	68.6	39.1	29.2
	$6*A1 + A14 + 2*A15 + 2*A11 + A12 + 3*A10 + 2*A17 + A16 + A38 + A53 + A7$					[373]
$\text{C}_{19}\text{H}_{27}\text{NO}_4^*$	3-[(hydroxyimino)(4-ethoxyphenyl)methyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
401.0	36.75		91.65	81.9	36.8	32.8
	$5*A1 + A14 + 2*A15 + 2*A12 + 4*A10 + 2*A17 + A16 + A38 + A32 + A2 + A7 + A53$					[373]
$\text{C}_{19}\text{H}_{27}\text{NO}_5^*$	3-[(hydroxyimino)(3,4-dimethoxyphenyl)methyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
393.0	36.20		92.1	82.2	36.2	32.3
	$6*A1 + A14 + 2*A15 + 3*A12 + 3*A10 + 2*A17 + A16 + A38 + 2*A32 + A7 + A53$					[373]
$\text{C}_{19}\text{H}_{38}\text{O}_2^*$	ethyl margarate (ethyl heptadecanoate)					
291.2	16.57	55.5				
298.4	36.2	115.7	171.2	189.5	52.8	56.6
	$2*A1 + A2 + 15A2*B2 + A38$					[391]
$\text{C}_{20}\text{H}_{13}\text{NO}_4$	1-amino-4-hydroxy-2-phenoxy-9,10-anthracenedione					
458.2	30.79		67.2	82.9	30.8	38.0
	$A14 + 3*A15 + 10*A10 + 4*A12 + A31 + A45 + A32 + 2*A114 + 4*A19$					[315]
$\text{C}_{20}\text{H}_{17}\text{F}_{25}^*$	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafuoroicosane					
192	2.4	12.5				
329	6.1	19.45				
361	23.7	65.65	97.6	467.7	32.5	166.1

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

<i>T</i> (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
324.2	5.60	17.27				[17]
355.2	21.90	61.66	78.93	467.7	27.50	166.1
	12*A4*B4 + 3*A25 + 22*A26 + A1 + 7*A2					
	Amphiphillic compound (values represent two sets of independent measurements)					
$\text{C}_{20}\text{H}_{17}\text{N}_3\text{O}_4^*$	4,11-diamino-2-butyl-1H-naphth[2,3-f]isoindole-1,3,5,10(2H)-tetraone					
490.2	24.85		50.69		24.85	[68]
	No prediction made (reporting authors express concern that the enthalpy is too small)					
$\text{C}_{20}\text{H}_{19}\text{BrS}^*$	2- <i>n</i> -butyl-5-(4-bromobiphenyl-4-yl)thiophene					
501.4	21.40		42.7	101.5	21.4	[315]
	A1 + 3*A2 + 8*A10 + 4*A12 + A21 + A14 + 2*A15 + A131 + 2*A19 + 2*A18					
$\text{C}_{20}\text{H}_{21}\text{F}_{21}^*$	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosafuoroicosane					
317	4.0	12.62				[14]
337	24.4	72.38	85.0	186.6	28.4	62.8
306.5	2.20	7.18				[17]
336.7	26.70	79.30	86.5	186.6	28.9	62.8
	10*A4*B4 + 3*A25 + 18*A26 + A1 + 9*A2					
	(Values represent two sets of independent measurements) Amphiphillic compound					
$\text{C}_{20}\text{H}_{21}\text{F}_{19}\text{O}^*$	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-nonadecafluoro-10-eicosanone					
317.9	53.17		167.3	181.4	53.2	57.7
	9*A4*B4 + 3*A25 + 16*A26 + A35 + A1 + 9*A2					
	Amphiphillic compound					
$\text{C}_{20}\text{H}_{23}\text{F}_{19}\text{O}^*$	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-nonadecafluoro-10-eicosanol					
346.2	3.60	10.40				[24]
356.0	33.50	94.10	104.5	184.6	37.1	69.2
	9*A4*B4 + 3*A25 + 16*A26 + A1 + 9*A2 + A30*B30 + A3*B3					
	Amphiphillic compound					
$\text{C}_{20}\text{H}_{24}$	8-(4-biphenyl)-1-octene					
291.5	21.00		72.0	107.2	21.0	31.3
	9*A20 + 2*A12 + A11 + 6*A2 + A5 + A6					
$\text{C}_{20}\text{H}_{24}\text{O}_6$	dibenzo[18-crown-6]					
435.75	57.46		131.9	106.1	57.5	44.1
	A14 + 15*A15 + 6*A112 + 4*A19 + 8*A10					
$\text{C}_{20}\text{H}_{26}\text{O}_3$	1,2,2-trimethyl-3-[(5,6,7,8-tetrahydro-2-naphthalenyl)carbonyl]cyclopentanecarboxylic acid					
421.3	22.94		54.5	65.1	22.9	27.4
	3*A1 + 2*A14 + 5*A15 + 2*A17 + A16 + 2*A19 + 3*A10 + A12 + A36*B36 + A35					
$\text{C}_{20}\text{H}_{28}\text{O}_5$	3-(3,4-diethoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
389.3	29.07		74.7	103.0	29.1	40.1
	5*A1 + A14 + 2*A15 + 2*A17 + A16 + 4*A10 + 2*A2 + 2*A12 + A36*C36 + A35 + 2*A32					
$\text{C}_{20}\text{H}_{32}\text{O}_4$	2,5-di- <i>n</i> -heptyloxy-1,4-benzoquinone					
275.8	3.6	13.05				[366]
372.5	17.3	46.44				[366]
406.2	38.4	94.53	154.0	140.8	59.3	57.2
	2*A1 + 12*A2 + A14 + 3*A15 + 2*A18*B18 + 2*A19 + 2*A32 + 2*A114					
$\text{C}_{20}\text{H}_{40}\text{O}_2^*$	methyl nonadecanoate					
304.2	19.4	63.7				[342]
313.2	42.8	136.8	200.5	189.5	62.2	56.6
	2*A1 + 17*A2*B2 + A38					
$\text{C}_{20}\text{H}_0\text{O}_4$	2,2,12,12-tetramethyl-1,3,11,13-tetraoxycycloicosane					
369.5	45.60		123.4	102.3	45.6	37.8
	4*A1 + A14 + 17*A15 + 2*A17 + 4*A112					
$\text{C}_{20}\text{H}_{42}\text{O}_{10}$	1, ω -dimethoxynona(oxyethylene)					
289.2	73.9		255.6	249.7	73.9	62.5
	2*A1 + 18*A2*B2 + 10*A32					
$\text{C}_{20}\text{H}_{43}\text{AsO}_2^*$	di- <i>n</i> -decylarsinic acid					
380	24.5	64.4				[386]
400	42.3	105.9	170.2	178.6	66.8	71.4
	2*A1 + 18*A2*B2 + A142					
$\text{C}_{20}\text{H}_{50}\text{Si}_5$	decaethylcyclopentasilane					
254.8	16.3	63.97				[381]
440.1	1.40	3.18	67.2	114.3	17.7	50.3
	10*A1 + 10*A2 + A14 + 2*A15 + 5*A139					
$\text{C}_{20}\text{H}_{60}\text{O}_{10}\text{Si}_{10}$	eicosanomethylcyclodecasiloxane					
265.8	39.76		149.6	113.3	39.8	30.1
	20*A1 + 10*A139 + 10*A112 + A14 + 17*A15					
$\text{C}_{21}\text{H}_{20}\text{BrN}_7\text{O}_6$	N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-[(2-cyanoethyl)-2-propenylamino]-					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
465.2	4-methoxyphenyl] acetamide					
	59.08		127.0	99.7	59.1	46.4
$\text{C}_{21}\text{H}_{20}\text{N}_4\text{O}_3^*$	4-methoxy-N,N-bis(3-pyridinylmethyl)-1,3-benzenedicarboxamide					
	28.43		70.4	101	28.4	40.8
403.9	11*A10+2*A11+3*A12+2*A41+2*A2+2*A60+A1+A32					
						392
$\text{C}_{21}\text{H}_{25}\text{F}_{19}^*$	1,1,1,2,3,3,4,4,5,5,6,6,7,7,8,8-hexadecafluoro-(trifluoromethyl)eicosane					
	34.00		109.6	177.7	34.0	55.1
$\text{C}_{21}\text{H}_{29}\text{NO}_3^*$	9*A4*B4+6*A25+A27+12*A26+A1+11*A2					
						22
425.0	3-[(hydroxyimino)(5,6,7,8-tetrahydro-2-naphthalenyl)methyl-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
	38.37		90.3	72.5	38.4	30.8
$\text{C}_{21}\text{H}_{30}\text{O}$	4*A1+2*A14+5*A15+3*A10+2*A19+2*A17+A12+A16+A38+A7+A53					
						373
404.7	1,1'-diadamantyl ketone					
	5.90	14.57				
470.0	6*A14+2*A15+6*A16+2*A17+A35					
	15.70	33.40	48.0	55.0	21.6	25.9
$\text{C}_{21}\text{H}_{40}$	<i>trans</i> -2-heptyl-6-butyldecalin					
	31.80		107.7	121.9	31.8	36.0
295.3	2*A14+4*A15+4*A16+2*A1+9*A2					
						40
$\text{C}_{21}\text{H}_{40}$	<i>trans</i> -2-propyl-6-octyldecalin					
	41.00		133.0	121.9	41.0	37.6
$\text{C}_{21}\text{H}_{42}\text{O}_2^*$	2*A14+4*A15+4*A16+2*A1+9*A2					
						40
300.2	ethyl nonadecanoate					
	18.49	61.6				
309.2	2*A1+A2+17*A2*B2+A38					
	43.18	139.7	201.3	189.5	61.7	56.6
$\text{C}_{21}\text{H}_{42}\text{O}_2^*$	methyl eicosanoate					
	73.7		231	210	73.7	61.7
319.2	2*A1+18*A2*B2+A38					
						391
$\text{C}_{21}\text{H}_{43}\text{NO}$	N-propylstearamide					
	16.02	46.03				
348.0	2*A1+16*A2*B2+A60+2A2					
	50.04	141.4	187.4	199.7	66.1	70.7
354.0	N-heptylmyristamide					
	6.54	20.70				
$\text{C}_{21}\text{H}_{43}\text{NO}$	2*A1+18*A2*B2+A60					
	49.02	142.9	163.6	204.1	55.6	70.0
316.0	N-decylundecanamide					
	0.07	0.21				
344.0	2*A1+18*A2*B2+A60					
	42.45	123.4	123.6	204.1	42.5	70.2
$\text{C}_{21}\text{H}_{43}\text{NO}$	N-laurylnonanamide					
	0.17	0.52				
328.0	2*A1+18*A2*B2+A60					
	66.91	196.2	196.7	204.1	67.1	69.6
341.0	N-myristylheptanamide					
	2.08	6.65				
$\text{C}_{21}\text{H}_{43}\text{NO}$	2*A1+18*A2*B2+A60					
	52.68	157.7	164.4	204.1	54.8	68.2
313.0	N-stearylpropanamide					
	1.84	5.45				
350.0	2*A1+17*A2*B2+A60+A2					
	56.03	160.1	165.6	201.9	57.9	70.7
$\text{C}_{22}\text{H}_{21}\text{F}_{25}^*$	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafuorodocosane					
	1.0	4.83				
207						
	9.5	27.78				
342						
	25.8	70.68	103.3	206.3	36.3	75.3
365						
						17
339.2	12*A4*B4+3*A25+22*A26+A1+9*A2					
	7.50	22.11				
357.2	22.20					
		62.15	84.26	206.3	29.7	73.7
$\text{C}_{22}\text{H}_{24}\text{O}_3^*$	Amphiphillic compound (values represent two sets of independent measurements)					
						68
444.2	3-([1,1-biphenyl]-4-ylcarbonyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	27.69		62.3	74.6	27.7	33.1
$\text{C}_{22}\text{H}_{25}\text{F}_{21}^*$	3*A1+A14+2*A15+2*A17+A16+9*A10+3*A12+A36*B36+A35					
						366
334.1	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosofluorodocosane					
	6.00	17.96				
338.1						
	27.00	79.86	97.8	200.8	33.0	67.9

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

<i>T</i> (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
	10*A4*B4 + 18*A26 + 3*A25 + A1 + 11*A2					[22]
	Amphiphillic compound					
C ₂₂ H ₂₆ N ₂ O ₂	(4R, 4'R, 5R, 5'R)-5,5-diphenyl-3,3',4,4'-tetramethyl-2,2'-bioxazolidine					
394.0	31.9		81.0	82.4	31.9	32.5
	2*A14 + 4*A15 + 2*A112 + 2*A119 + 6*A16 + 4*A1 + 10*A10 + 2*A11					[387]
C ₂₂ H ₂₆ N ₂ O ₂	(2R, 3R, 6R, 7R)-2,6-diphenyl-3,4,7,8-tetramethyl-cis-perhydro-[1,4]-oxazino-[3,2- <i>b</i>]-[1,4]-oxazine					
379.4	18.4		48.5	82.4	18.4	31.3
	2*A14 + 4*A15 + 2*A112 + 2*A119 + 6*A16 + 4*A1 + 10*A10 + 2*A11					[387]
C ₂₂ H ₂₈ N ₂ O	N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]propanamide (fentanyl)					
357.2	22.51		63.0	84.6	22.5	30.2
	A14 + 3*A15 + A16 + A119 + 3*A2 + 10*A10 + A11 + A12 + A1 + A125					[296]
C ₂₂ H ₂₉ NO ₂	4- <i>n</i> -octyloxy-N-(4-methoxybenzylidene)aniline					
377.3	42.29		112.1	127.0	42.3	47.9
	2*A1 + 7*A2 + 2*A32 + 8*A10 + 4*A12 + A6 + A42					[141]
C ₂₂ H ₃₀ N ₂ O ₂ S	N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenylpropanamide (sufentanil)					
370.2	23.85		64.4	102.3	23.9	37.9
	2*A14 + 5*A15 + A17 + A119 + A59 + 5*A10 + A12 + 2*A1 + 4*A2 + A32 + 2*A18 + A18*B18 + A19 + A131					[296]
C ₂₂ H ₃₆ O ₄	2,5-di- <i>n</i> -octyloxy-1,4-benzoquinone					
358.2	9.4	26.24				
405.8	43.0	106.0	132.2	155.0	52.4	62.9
	2*A1 + 14*A2 + A14 + 3*A15 + 2*A18*B18 + 2*A19 + 2*A32 + 2*A114					[342]
C ₂₂ H ₄₀ O ₂	3,3,6,6,10,10,13,13-octamethylcyclotetradecane-1,8-dione					
492.2	24.7		50.2	73.7	24.7	36.3
	8*A1 + 4*A17 + 2*A114 + A14 + 11*A15					[115]
C ₂₂ H ₄₆ O	1-docosanol					
333.9	17.24	50.72				
345.2	46.57	134.9	185.6	214.6	63.8	74.08
	A1 + 21*A2*B2 + A30					[88]
C ₂₂ H ₄₇ AsO ₂ *	di- <i>n</i> -undecylarsinic acid					
384	30.0	78.2				
396	45.1	113.9	192.1	197.2	75.1	78.1
	2*A1 + 20*A2*B2 + A142					[381]
C ₂₂ H ₆₆ O ₁₁ Si ₁₁	docosamethylcycloundecasiloxane					
216.2	17.73		82.0	122.4	17.7	26.5
	22*A1 + 11*A139 + 11*A112 + A14 + 19*A15					[121]
C ₂₃ H ₂₄ N ₆ O ₄	2-[[4-[(2-acetoxy)ethyl]butylamino]-2-methylphenyl]azo]-5-nitro-1,3-benzenedicarbonitrile					
424.2	37.88		89.3	105.7	37.9	44.8
	5*A10 + 6*A12 + A11 + 2*A56 + A50 + 3*A1 + 5*A2 + 2*A42 + A43 + A38					[315]
C ₂₃ H ₂₅ BrN ₆ O ₁₀	N-[5-[bis[(2-acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]acetamide					
421.2	57.28		136.0	117.1	57.3	49.3
	4*A10 + 8*A12 + 4*A1 + 4*A2 + 2*A38 + A21 + 2*A50 + 2*A42 + A32 + A60 + A43					[315]
C ₂₃ H ₃₁ NO	4- <i>n</i> -octyloxy-N-(3,5-dimethylbenzylidene)aniline					
324.7	37.7		116.2	120.8	37.7	39.2
	3*A1 + 7*A2 + A32 + 7*A10 + 2*A11 + 3*A12 + A6 + A42					[141]
C ₂₃ H ₃₁ NO ₃	4- <i>n</i> -octyloxy-N-(3,5-dimethoxybenzylidene)aniline					
316.3	35.3		111.6	134.4	35.3	42.5
	3*A1 + 7*A2 + 3*A32 + 7*A10 + 5*A12 + A6 + A42					[141]
C ₂₃ H ₄₄	<i>trans</i> -2-heptyl-6-hexyldecalin					
312.2	38.9		124.6	136.1	38.9	42.5
	2*A1 + 4*A15 + 4*A16 + 2*A1 + 11*A2					[40]
C ₂₃ H ₄₄	<i>trans</i> -2-pentyl-6-octyldecalin					
314.2	43.5		138.5	136.1	43.5	42.8
	2*A1 + 4*A15 + 4*A16 + 2*A1 + 11*A2					[40]
C ₂₃ H ₄₆ O ₂ *	methyl behenate (methyl docosanoate)					
327.2	82.3		231	210	82.3	67.1
	2*A1 + 20A2*B2 + A38					[391]
C ₂₄ H ₁₈ N ₂ S ₂ *	4,4'-bis-(2-thienylmethylideneamino)- <i>trans</i> -stilbene					
567.2	44.90	79.16				
580.2	0.20	0.34	79.5		45.1	
	No prediction made (forms liquid crystal)					[86]
C ₂₄ H ₁₈ N ₂ S ₂ *	1,2-bis-[5-(β -azastyryl)-2-thienyl]- <i>trans</i> -ethylene					
501.2	45.90		91.6	108.4	45.9	54.3
	10*A10 + 2*A12 + 4*A6 + 2*A42 + 2*A14 + 4*A15 + 4*A18 + 4*A19 + 2*A131					[86]
C ₂₄ H ₂₅ F ₂₅ *	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorotetracosane					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (calcd)
352.1	10.00	28.40				
364.1	26.00	71.41	99.8	220.5	36.0	80.3
	12*A4*B4+3*A25+22*26+A1+11*A2					
	Amphiphillic compound					
	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluoro-14-methyltricosane					
C ₂₄ H ₂₅ F ₂₅ *	9.00	34.61				[22]
220.0	25.00	72.02	106.6	207.5	34.0	72.0
347.1	12*A4*B4+3*A25+22*A26+2*A1+A3+9*A2					
	Amphiphillic compound					
	2,2'-diphenyl-bi(5,5-dimethyl-1,3-dioxan-2-yl)					
C ₂₄ H ₃₀ O ₄	49.8		98.2	80.6	49.8	40.9
507.1	2*A14+6*A15+4*A17+4*A112+10*A10+2*A11+4*A1					
	8-[4-(4'- <i>n</i> -butylbiphenyl)]-1-octene					
C ₂₄ H ₃₂ *	2.20	8.85				[385]
248.6	9.60	30.4	39.3	129.1	11.8	40.7
315.6	8*A10+2*A12+2*A11+A5+A6+A1+9*A2					
	Forms liquid crystal					
	2,5-di- <i>n</i> -nonyloxy-1,4-benzoquinone					
C ₂₄ H ₄₀ O ₄	8.0	22.69				
352.6	24.2	63.05				
383.8	47.1	117.0	202.7	169.2	79.3	68.1
402.7	2*A1+16*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114					
	dibenzo[24-crown-8]					
C ₂₄ H ₄₀ O ₈	16.6	46.9				[342]
354.1	52.25	139.2	186.1	130.1	68.85	49.1
375.4	A14+15*A15+6*A112+4*A19+8*A10					
	<i>trans</i> -2,6-diheptyldecalin					
C ₂₄ H ₄₄	40.17		123.0	143.2	40.2	46.8
326.7	2*A1+4*A15+4*A16+2*A1+11*A2					
	3,3,7,7,11,11,15,15-octamethylcyclohexadecane-1,9-dione					
C ₂₄ H ₄₄ O ₂	34.30		81.0	81.1	34.3	34.3
423.2	8*A1+4*A17+2*A114+A14+13*A15					
	2-(docosanoxy)ethanol					
C ₂₄ H ₅₀ O ₂ *	12.92	40.73				[115]
317.2	43.93	130.8	171.5	249.5	56.9	83.8
335.9	A1+21*A2*B2+A32+A30*B30					
	di- <i>n</i> -dodecylarsinic acid					
C ₂₄ H ₅₁ AsO ₂ *	31.4	81.5				[88]
385	49.4	124.1	205.7	215.8	80.8	85.9
398	2*A1+22*A2*B2+A142					
	tetracosamethylcyclododecasiloxane					
C ₂₄ H ₇₂ O ₁₂ Si ₁₂	15.45		65.97	131.5	15.5	30.8
234.2	24*A1+12*A139+12*A112+A14+21*A15					
	1,2-bis-[5-(4-methoxy- β -azastyryl)-2-thienyl]- <i>trans</i> -ethylene					
C ₂₆ H ₂₂ N ₂ O ₂ S ₂ *	63.50	118.0				[121]
538.2	0.80	1.41	119.4	123.2	64.30	69.88
567.2	2*A1+8*A10+4*A12+4*A6+2*A42+2*A14+4*A15+4*A18+4*A19+2*A131+2*A32					
	Forms liquid crystal					
	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafuoroheptacosane					
C ₂₆ H ₂₉ F ₂₅ *	16.3	44.90				[86]
363	26.1	71.31	116.2		42.4	
366						[17]
359.2	26.0	72.38			26.0	
	Amphiphillic compound (values represent two sets of independent measurements)					
	<i>trans</i> -1-(4-heptanoylphenyl)-4-heptylcyclohexane					
C ₂₆ H ₄₂ O*	16.49	48.05				[68]
343.2	7.71	22.37	70.4	145.5	24.2	50.2
344.7	A14+3*A15+2*A16+4*A10+A11+A12+2*A1+11*A2+A35					
	Forms liquid crystal					
	4,4,7,7,13,13,16,16-octamethylcyclooctadecane-1,10-dione					
C ₂₆ H ₄₈ O ₂	50.60		102.8	88.5	50.6	43.6
492.2	8*A1+4*A17+2*A114+A14+15*A15					
	1-hexacosanol					
C ₂₆ H ₅₄ O	16.74	50.39				[115]
332.2	67.78	192.7	243.1	251.8	84.5	88.6
351.7	A1+25*A2*B2+A30					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (calcd)
$\text{C}_{26}\text{H}_{55}\text{AsO}_2^*$	di- <i>n</i> -tridecylarsinic acid					
388	36.5	94.0				
396	52.7	133.1	227.2	234.4	89.2	92.8 [381]
$\text{C}_{27}\text{H}_{42}\text{Cl}_2\text{N}_2\text{O}_6^*$	2*A1 + 24*A2*B2 + A142 chloramphenicol palmitate polymorph A					
367.3	51.04	0	139	188.6	51.04	69.2
	chloramphenicol palmitate polymorph B					
360.8	41.3	0	112.5	188.6	41.3	69.2
	4*A10 + A11 + A12 + A50 + A30*F30 + 2*A22*F22 + A60 + A38 + A2 + 3*A3*B3 + A1 + 14*A2					
						[395]
$\text{C}_{28}\text{H}_{22}\text{N}_2\text{O}_2$	1,4-[bis[(4-methylphenyl)amino]-9,10-anthracenedione					
491.2	36.59	74.5		71.5	36.6	35.1 [315]
	3*A15 + A14 + 14*A10 + 4*A19 + 2*A114 + 4*A12 + 2*A11 + 2*A44					
$\text{C}_{28}\text{H}_{31}\text{F}_{25}^*$	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorooctacosane					
263.2	43.10		163.8	248.9	43.10	65.5 [68]
	12*A4*B4 + 3*A25 + 22*A26 + A1 + 15*A2					
$\text{C}_{28}\text{H}_{48}\text{O}^*$	Amphiphilic compound <i>trans</i> -1-heptyl-4-(4-nonanoylphenyl)cyclohexane					
343.4	20.8	60.6				
353.3	11.32	32.1	92.6	159.7	32.1	56.4
	A14 + 3*A15 + 2*A16 + 4*A10 + A11 + A12 + 2*A1 + 13*A2 + A35					
	Forms liquid crystal					
						[25]
$\text{C}_{28}\text{H}_{48}\text{O}_4$	2,5-di- <i>n</i> -undecyloxy-1,4-benzoquinone					
367.4	12.9	35.11				
390.0	28.4	72.8				
397.2	52.1	131.2	239.1	241.6	93.4	96.0 [342]
	2*A1 + 20*A2*B2 + A14 + 3*A15 + 2*A18*B18 + 2*A19 + 2*A32 + 2*A114					
$\text{C}_{28}\text{H}_{52}\text{O}_2$	4,4,8,8,14,14,18,18-octamethylcycloeicosane-1,11-dione					
418.2	36.80	88.0		95.9	36.8	40.1 [115]
	8*A1 + 4*A17 + 2*A114* + A14 + 17*A15					
$\text{C}_{28}\text{H}_{59}\text{AsO}_2^*$	di- <i>n</i> -tetradecylarsinic acid					
390	39.3	100.6				
397	58.2	146.6	247.2	253.0	97.5	100.5 [381]
	2*A1 + 26*A2*B2 + A142					
$\text{C}_{29}\text{H}_{41}\text{NO}_4$	17-(cyclopropylmethyl)- α -(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro- 6-methoxy- α -methyl-6,14-ethenomorphinan-7-methanol					
491.3	26.80		54.55	68.6	26.80	33.7
	6*A14 + 2*A15 + 5*A1 + 2*A4 + A30*E30 + 4*A16 + 3*A17 + A119 + A112 + A31 + A32 + 3*A19 + A12 + 2*A10 + A2					
						[320]
$\text{C}_{30}\text{H}_{37}\text{F}_{25}^*$	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorotricontane					
365.2	47.80		130.9	263.1	47.80	96.1 [68]
	12*A4*B4 + 3*A25 + 22*A26 + A1 + 17*A2					
$\text{C}_{30}\text{H}_{56}\text{O}_2$	5,5,8,8,16,16,19,19-octamethylcyclodocosane-1,12-dione					
442.2	47.70	107.9		95.9	47.7	42.4 [115]
	8*A1 + 4*A17 + 2*A114 + A14 + 17*A15					
$\text{C}_{30}\text{H}_{60}\text{O}_{15}$	45-crown-15					
311.2	70.6		227	206.8	70.6	64.3 [386]
	A14 + 42*A15 + 15*A112					
$\text{C}_{30}\text{H}_{63}\text{AsO}_2^*$	di- <i>n</i> -pentadecylarsinic acid					
390	46.4	119				
396	63.6	160.5	279.6	271.6	110.0	107.6 [381]
	2*A1 + 28*A2*B2 + A142					
$\text{C}_{31}\text{H}_{43}\text{NO}_5$	3-(acetyloxy)-17-(cyclopropylmethyl)- α -(1,1-dimethylethyl)-4,5-epoxy- 18,19-dihydro-6-methoxy- α -methyl-6,14-ethenomorphinan-7-methanol					
440.3	22.40		50.9	68.9	22.4	30.3 [320]
	6*A14 + 2*A15 + 6*A1 + 2*A4 + A30*E30 + 4*A16 + 3*A17 + A119 + A112 + 3*A19 + A12 + 2*A10 + A2 + A38					
$\text{C}_{32}\text{H}_{34}$	1,8-bis-(4-biphenyl)octane					
415.2	56.00		134.9	140.8	56.0	58.5 [97]
	18*A10 + 4*A12 + 2*A11 + 8*A2					
$\text{C}_{32}\text{H}_{34}^*$	1,8-bis[4(4'-ethylbiphenyl)]butane					
454.2	46.00		101.3	127.8	46.0	58.1 [97]
	2*A1 + 6*A2 + 16*A10 + 4*A12 + 4*A11					
$\text{C}_{32}\text{H}_{41}\text{F}_{25}^*$	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosofluorodotriacontane					
369.2	43.40		117.6	277.3	43.4	102.3 [68]
	12*A4*B4 + 3*A25 + 22*A26 + A1 + 19*A2					
$\text{C}_{32}\text{H}_{64}\text{16}$	48-crown-16					
312.2	59.1		189.4	219.1	59.1	68.4 [386]
	A14 + 45*A15 + 16*A112					

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

<i>T</i> (K)	ΔH_{pcc} (expt)	ΔS_{pcc} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpcc}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpcc}}$ (calcd)	
C ₃₂ H ₄₅ NO ₅	410.2	17-(cyclopropylmethyl)- α -(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy- α -methyl-(1-oxopropoxy)-6,14-ethenomorphinan-7-methanol					
		27.10		66.07	76.0	27.10	31.2
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+3*A19+A12+2*A10+2*A2+A38					
						[320]	
C ₃₂ H ₆₀ O ₂	380.2	5,5,9,9,17,17,21,21-octamethylcyclotetracosane-1,13-dione					
		32.60		85.7	110.7	32.6	42.1
		8*A1+4*A17+2*A114+A14+21*A15					
		di- <i>n</i> -hexadecylarsinic acid					
C ₃₂ H ₆₇ AsO ₂ *	389	47.4	121.9			[115]	
	395	66.8	169.2	291	290.2	114.2	114.6
		2*A1+30*A2*B2+A142					
		[381]					
C ₃₃ H ₄₇ NO ₅	422.1	17-(cyclopropylmethyl)- α -(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy- α -methyl-(1-oxobutoxy)-6,14-ethenomorphinan-7-methanol					
		32.40		76.76	83.1	32.40	35.1
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+3*A19+A12+2*A10+3*A2+A38					
						[320]	
C ₃₄ H ₃₁ ClN ₂ O ₃ *	442.2	spiro[isobenzofuran-1(3H),9'(9H)-7'-chloro-6'-(methylcyclohexylamino)-3'-methyl-2'-anilinoxanthene]-3-one					
		49.0		110.8	91.5	49.0	40.5
		3*A14+8*A15+2*A1+13*A10+4*A12+A11+6*A19+A16+A17+A112+A115+A43+A44+A22*E22					
						[371]	
C ₃₄ H ₃₂ N ₂ O ₃	476.2	spiro[isobenzofuran-1(3H),9'(9H)-6'-(methylcyclohexylamino)-3'-methyl-2'-anilinoxanthene]-3-one					
		39.9		83.8	90.2	39.9	43.0
		3*A14+8*A15+2*A1+14*A10+3*A12+A11+6*A19+A16+A17+A112+A115+A43+A44					
						[371]	
C ₃₄ H ₃₈ *	393.2	1,6- <i>bis</i> -[4-(4'-ethylbiphenyl)]hexane					
	422.2	3.90	9.92				
		35.00	82.90	92.83	142.0	38.9	60.0
		2*A1+8*A2+16*A10+4*A11+4*A12					
						[97]	
C ₃₄ H ₄₉ NO ₅	379.1	17-(cyclopropylmethyl)- α -(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy- α -methyl-(1-oxopentoxo)-6,14-ethenomorphinan-7-methanol					
		24.00		63.31	90.2	24.0	34.2
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+3*A19+A12+2*A10+4*A2+A38					
						[320]	
C ₃₄ H ₆₈ O ₁₇	301.2	51-crown-17					
		66.6		221.1	231.4	66.6	69.7
		A14+48*A15+17*A112					
						[386]	
C ₃₄ H ₇₁ AsO ₂ *	390	di- <i>n</i> -octadecylarsinic acid					
	393	50.9	130.6				
		68.6	174.5	305.1	308.8	119.5	121.4
		2*A1+32*A2*B2+A142					
		[381]					
C ₃₅ H ₅₁ NO ₅	352.6	17-(cyclopropylmethyl)- α -(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy- α -methyl-(1-oxohexyloxy)-6,14-ethenomorphinan-7-methanol					
		22.60		64.1	97.3	22.6	35.0
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+3*A19+A12+2*A10+5*A2+A38					
						[320]	
C ₃₆ H ₄₂ *	402.2	1,8- <i>bis</i> -[4-(4'-ethylbiphenyl)]octane					
	413.2	8.40	20.89				
		42.00	101.6	122.5	156.2	50.4	64.5
		2*A1+16*A10+4*A12+4*A11+10*A2					
						[97]	
C ₃₆ H ₄₂ *	404.2	1,4- <i>bis</i> -[4-(4'- <i>n</i> -butylbiphenyl)]butane					
	464.2	12.00	29.68				
		24.00	51.70	81.3	142.0	36.0	60.0
		2*A1+16*A10+4*A12+4*A11+10*A2					
		Forms liquid crystal					
						[97]	
C ₃₆ H ₅₃ NO ₅	360.0	17-(cyclopropylmethyl)- α -(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy- α -methyl-(1-oxoheptyloxy)-6,14-ethenomorphinan-7-methanol					
		19.30		53.61	104.4	19.30	37.6
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+3*A19+A12+2*A10+6*A2+A38					
						[320]	
C ₃₆ H ₆₄ O ₄	385.9	2,5-di- <i>n</i> -pentadecyloxy-1,4-benzoquinone					
	393.5	21.7	56.23				
		101.7	258.5	314.7	316.0	123.4	124.3
		2*A1+28*A2*B2+A14+3*A15+2*A18+2*A19+2*A32+2*A14					
						[342]	
C ₃₆ H ₇₄ O ₁₆	317.2	54-crown-18					
		81.6		257.2	243.7	81.6	77.3

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

<i>T</i> (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)	
C ₃₆ H ₇₄ O ₁₈	A14+51*A15+18*A112 1, ω -dimethoxyheptadeca(oxyethylene)						[386]
	301.2	136.6		453.5	436.2	136.6	
C ₃₆ H ₇₅ AsO ₂ *	2*A1+34*A2*B2+18*A32 di- <i>n</i> -nonadecylarsinic acid						[386]
	394	128.9		327.2	327.4	128.9	
C ₃₈ H ₆₈ O ₄	2*A1+34*A2*B2+A142 2,5-di- <i>n</i> -hexadecyloxy-1,4-benzoquinone						[381]
	357.7	6.8	18.73				
	370.9	14.1	38.02				
	389.0	19.0	48.84				
	394.2	83.0	210.6	316.1	334.6	122.9	
C ₃₈ H ₇₈ O ₁₉	2*A1+30*A2*B2+A14+3*A15+2*A18+2*A19+2*A32+2*A114 1, ω -dimethoxyoctadeca(oxyethylene)						[342]
	305.2	156.7		513.5	459.5	156.7	
C ₄₀ H ₄₀ N ₂ O ₄ *	2*A1+36*A2*B2+19*A32 3,3',4,4'-biphenyltetracarboxy-N,N'-bis-(4- <i>n</i> -hexylphenyl)diimide						[386]
	432.4	19.9	46.02				
	513.8	26.2	50.99				
	563.3	9.50	16.86	113.9		55.60	
C ₄₀ H ₅₀ *	No prediction made. Forms liquid crystal						[87]
	1,8-bis[4(4'- <i>n</i> -butylbiphenyl)]octane						
	398.2	13.0	32.65				
C ₄₀ H ₇₂ O ₄	2*A1+16*A10+4*A12+4*A11+14*A2 Forms liquid crystal						[97]
	414.2	27.0	65.19	97.2	184.6	40.0	
	2,5-di- <i>n</i> -heptadecyloxy-1,4-benzoquinone						
	383.6	13.0	33.89				
	395.3	120.9	305.8	339.7	353.1	133.9	
C ₄₂ H ₄₄ N ₂ O ₄ *	2*A1+32*A2*B2+A14+3*A15+2*A18+2*A19+2*A32+2*A114 3,3',4,4'-biphenyltetracarboxy-N,N'-bis-(4- <i>n</i> -heptylphenyl)diimide						[342]
	411.0	18.80	45.74				
	504.9	24.70	48.92				
	560.8	11.10	19.79	114.5		54.6	
	Forms liquid crystal						[87]
C ₄₄ H ₄₈ N ₂ O ₄ *	3,3',4,4'-biphenyltetracarboxy-N,N'-bis-(4- <i>n</i> -octylphenyl)diimide						
	428.5	36.10	84.25				
	499.2	21.30	42.67				
	553.5	8.50	15.36	142.3		65.9	
C ₄₄ H ₈₀ O ₄	Forms liquid crystal						[87]
	2,5-di- <i>n</i> -nonadecyloxy-1,4-benzoquinone						
	385.5	16.2	42.0				
	396.2	134.0	338.2	380.2	390.5	150.2	
C ₄₄ H ₉₀	2*A1+36*A2*B2+A14+3*A15+2*A18+2*A19+2*A32+2*A114 <i>n</i> -tetratetracontane						[342]
	360.9	145.5		403.1	425.8	145.5	
C ₅₀ H ₁₀₂	2*A1+42*A2*B2 <i>n</i> -pentacontane						[210]
	366.9	185.0		504.2	481.6	185.0	
C ₅₂ H ₁₀₆ O ₂₆	2*A1+48*A2*B2 1, ω -dimethoxypentacos(oxyethylene)						[210]
	316.2	209.7		663.3	622.7	209.7	
C ₅₄ H ₁₀₈ O ₂₇	2*A1+50*A2*B2+26*A32 81-crown-27						[386]
	314.2	155.6		495.4	354.4	155.6	
C ₅₆ H ₁₁₄ O ₂₈	A14+78*A15+27*A112 1, ω -dimethoxyheptacos(oxyethylene)						[386]
	315.2	224.6		712.6	669.3	224.6	
C ₉₂ H ₁₈₆ O ₄₆	2*A1+54*A2*B2+28*A32 1, ω -dimethoxypentatetracos(oxyethylene)						[386]
	324.2	374.8		1156.3	1089.0	374.8	
C ₁₀₀ H ₂₀₂	2*A1+90*A2*B2+46*A32 <i>n</i> -hectane						[386]
	365.5	54.8	149.9				
	388.5	331.8	854.1	1004.0	946.7	386.8	
C ₁₉₂ H ₃₈₆	2*A1+98*A2*B2 <i>n</i> -dononacontahectane						[343]

TABLE 7. Calculated and experimental phase change enthalpies and entropies of test solids—Continued

T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ (calcd)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (expt)	$\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ (calcd)
399.1	698.9		1751.2	1802.4	698.9	719.3
	2*A1 + 190*A2*B2 (Authors noted a small premelting transition)					[344]

^aUnits for $\Delta_0^{T_{\text{fus}}} S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}} H_{\text{tpce}}$ are $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ and $\text{kJ}\cdot\text{mol}^{-1}$, respectively; compounds with molecular formulas characterized with an asterisk(*) were not included in generating the statistics. As noted in the table, some of these compounds exhibit liquid crystal behavior, others display amphiphilic behavior, group values for some are not currently available, the error between experimental and calculated total phase change entropy exceeded three standard deviations or some may have been added at a later date.

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