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 ($\Delta_0^{T_{fus}}S_{tpce}$) and enthalpy ($\Delta_0^{T_{fus}}H_{tpce}$) 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 $J\cdot mol^{-1}\cdot K^{-1}$ and 3.52 $kJ\cdot mol^{-1}$, and 0.154 and 0.17 for $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$, respectively. For the 260 test compounds, standard deviations of $\pm 13.0\,J\cdot mol^{-1}\cdot K^{-1}$ ($\Delta_0^{T_{fus}}S_{tpce}$) and $\pm 4.88\,kJ\,mol^{-1}$ ($\Delta_0^{T_{fus}}H_{tpce}$) 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 molecular 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 $\Delta_{fus}H_m$, 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:

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

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

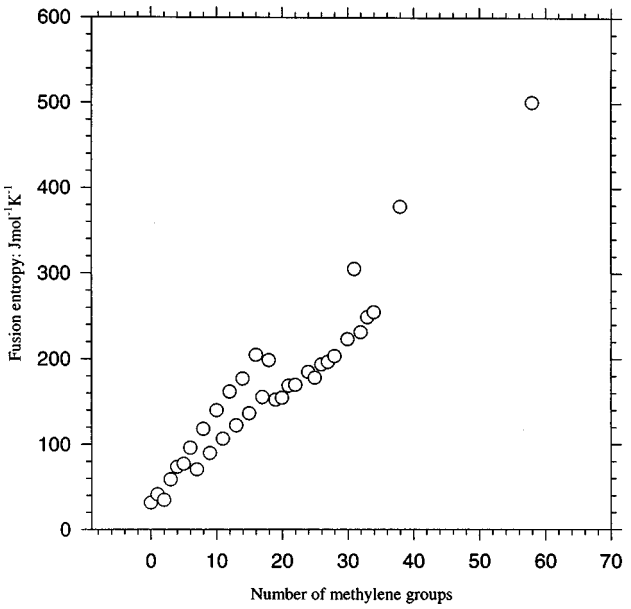


FIG. 1. Fusion entropy of the *n*-alkanes as a function of the number of methylene groups.

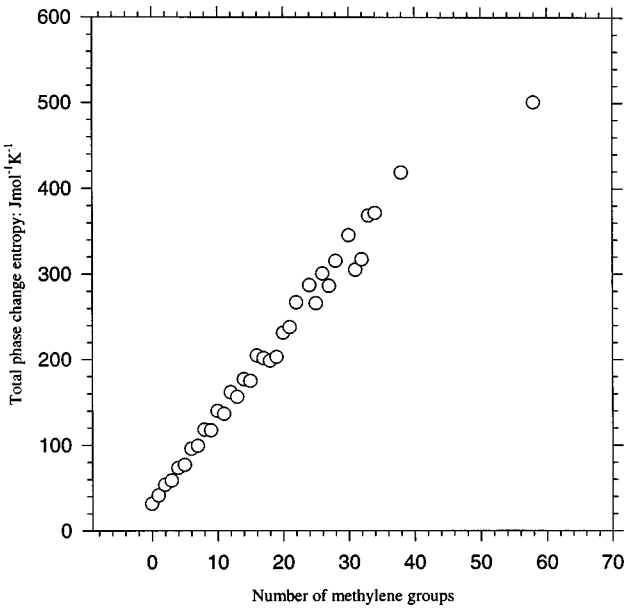


FIG. 2. Total phase change entropies of the *n*-alkanes as a function of the number of methylene groups.

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:

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

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

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 application of these parameters in the estimation of $\Delta_0^{T_{\rm fus}} S_{\rm tpce}$ and $\Delta_0^{T_{\rm fus}} H_{\rm tpce}$, 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 $\Delta_0^{T_{\rm fus}} S_{\rm tpce}$ 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 $\Delta_0^{T_{\rm fus}} S_{\rm tpce}$ 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 then 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, $C_{\rm CH_2}$, is applied differently from the rest and its application is discussed below. Introduction of this coefficient is new and differentiates this pro-

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

$$\Delta_0^{T_{fus}}S_{tpce}(aah)=\sum_i n_iG_i+n_{CH_2}C_{CH_2}G_{CH_2};$$

$$C_{CH_2}=1.31 \quad \text{when} \quad n_{CH_2}\geqslant\sum n_i;$$

$$i\neq CH_2 \quad \text{otherwise} \quad C_{CH_2}=1. \tag{2}$$

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 Σn_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_t 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 $\Delta_0^{T_{fus}}S_{tpce}$ and T_{fus} is followed by the experimental total phase change enthalpy (or fusion enthalpy). Finally, details in estimating $\Delta_0^{T_{fus}}S_{tpce}$ 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 $J\cdot mol^{-1}\cdot K^{-1}$ and together with the experimental melting point, an enthalpy of fusion of 12.6 $kJ\cdot mol^{-1}$ is estimated. This can be compared to the experimental value of 11.0 $kJ\cdot mol^{-1}$. 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 ($C_{CH_2}=1.0$) and would not be counted in Σn_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 acenaphtylene, according to this definition is not. Estimation of $\Delta_0^{T_{fus}}S_{tpce}$ for acenaphthylene will be illustrated below.

3.2. Nonaromatic Cyclic and Polycyclic Hydrocarbons

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

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

$$n=\text{number of ring atoms}, \tag{3}$$

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

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

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, $\Delta_0^{T_{fus}}S_{tpce}(corr)$. These correction terms can be found in Table 1(b). Once these corrections are included in the estimation, any additional acyclic groups present as substitutents on the ring are added to the results of Eqs. (3) or (4) and $\Delta_0^{T_{fus}}S_{tpce}(corr)$. These additional acyclic and/or aromatic terms $[\Delta_0^{T_{fus}}S_{tpce}(aah)]$ 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 $\Delta_0^{T_{fus}}S_{tpce}(total)$:

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

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

The estimation of $\Delta_0^{T_{fus}}S_{tpce}$ 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 $\Delta_0^{T_{fus}}S_{tpce}$ (*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), $\Delta_0^{T_{fus}}S_{tpce}$ (*corr*), completes the estimation.

3.2.3. Acenaphthylene

Estimation of $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ 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 $\Delta_0^{T_{fus}}S_{tpce}$ (*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 substitutents that may be present. In acenaphthylene, the contribution of the five membered ring $\{\Delta_0^{T_{fus}}S_{tpce}(ring):[33.4]+2[3.7]\}$ is first adjusted for each nonsecondary sp^3 carbon atom in the ring $\{\Delta_0^{T_{fus}}S_{tpce}(corr):+2[-1.6]+3[-12.3]\}$, and then the remainder of the aromatic portion of the molecule is added $\{\Delta_0^{T_{fus}}S_{tpce}(aah):[-7.5]+6[7.4]\}$. In a molecule such as [2,2]-*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), $\Sigma_i n_i C_i G_i$, and the contribution of the functional group(s) $\Sigma_k n_k C_j G_k$. 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 $\Delta_0^{T_{fus}}S_{tpce}(total)$ for acyclic and aromatic derivatives and for cyclic and polycyclic hydrocarbon derivatives, respectively,

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

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

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 trisubstituted 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 $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ 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 $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ 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 $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ 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 $\Delta_0^{T_{\rm fus}}S_{\rm tpce}(corr)$. 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 (–CONRCO–) and cyclic amide nitrogen (–NH–), a cyclic urea (–NRCONH–) and amide carbonyl (–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 (–NRCONH–, –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 $\Delta_0^{T_{fus}}S_{tpce}$ of small molecules, the parameters of Tables 1 and 2 can be used to predict $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ (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 $\Delta_0^{T_{fus}}S_{tpce}$ 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 $(CH_2O)_n$, is treated as an infinite chain with $n_0 = n_{CH_2}$. For a molecule such as $CH_3O(CH_2CH_2O)_nCH_3$, the number of methylene groups in the repeat unit exceeds the number of oxygens and therefor 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 instance 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 $\Delta_0^{T_{fus}}S_{tpce}$ 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 ambiquity 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 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]

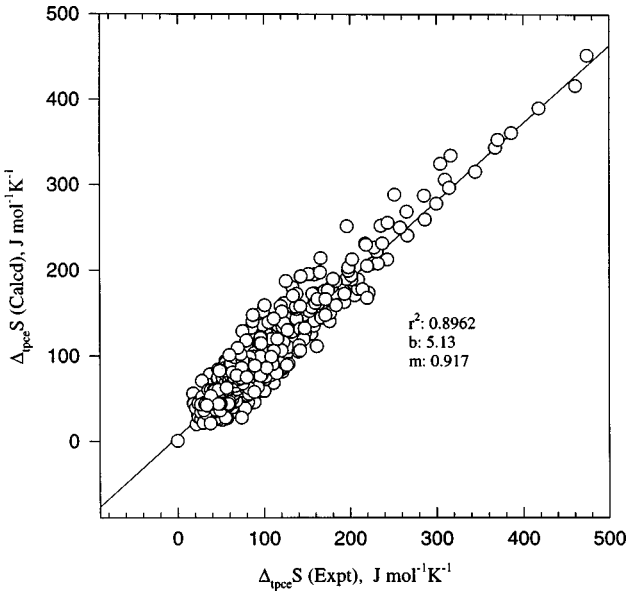


FIG. 3. A comparison of calculated and experimental $\Delta_0^{T_{fus}}S_{tpce}$ of 1858 database compounds.

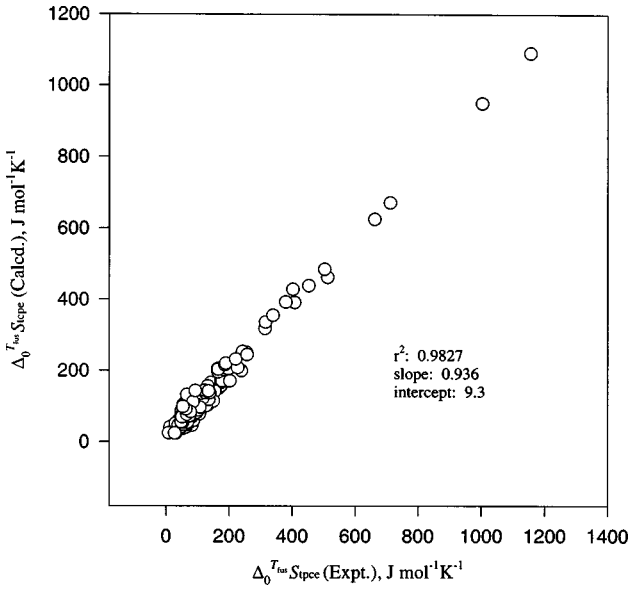


FIG. 5. A comparison of calculated and experimental $\Delta_0^{T_{fus}}S_{tpce}$ of 260 test compounds.

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 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

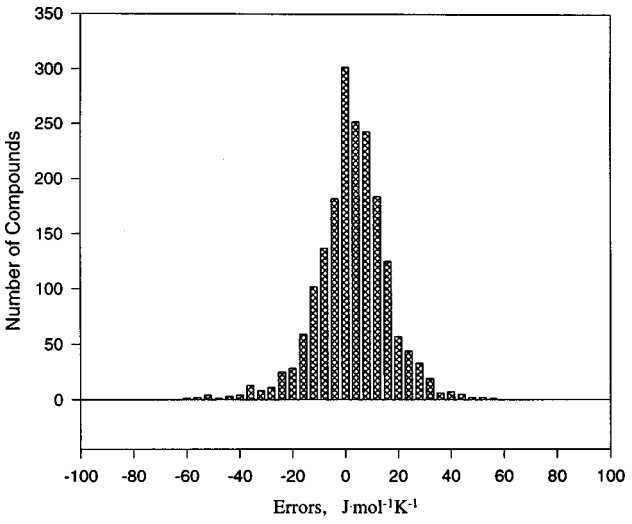


FIG. 4. A histogram illustrating the distribution of errors in estimating $\Delta_0^{T_{fus}}S_{tpce}$ of the database compounds.

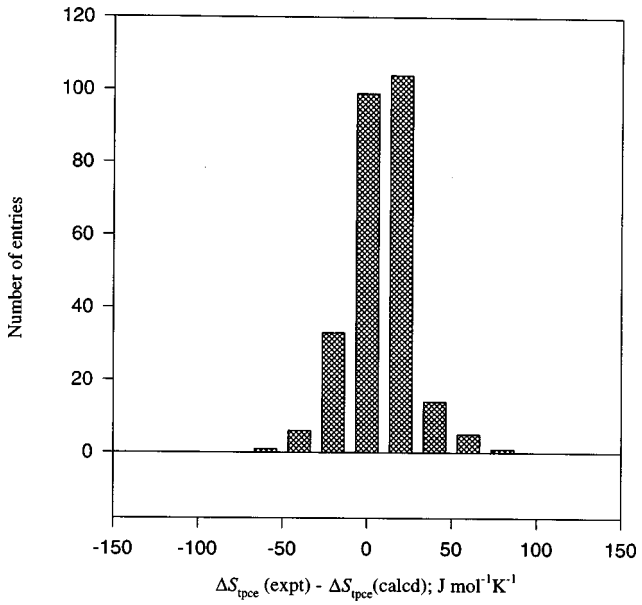


FIG. 6. A histogram illustrating the distribution of errors in estimating $\Delta_0^{T_{fus}}S_{tpce}$ of 260 test compounds.

calculated $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ values for these 1858 compounds are 9.9 $J\cdot mol^{-1}\cdot K^{-1}$ and 3.52 $kJ\cdot mol^{-1}$, and 0.154 and 0.17, respectively. The standard deviations between experimental and calculated values for $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ are $\pm 13.0\,J\cdot mol^{-1}\cdot K^{-1}$ and $\pm 4.88\,kJ\cdot mol^{-1}$, 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 $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ were $\pm 18.4\,J\cdot mol^{-1}\cdot K^{-1}$ and $\pm 7.2\,kJ\cdot mol^{-1}$, respectively. The absolute average and relative errors between experimental and calculated $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ values for these 260 compounds were 13.9 $J\cdot mol^{-1}\cdot K^{-1}$ and 5.28 $kJ\cdot mol^{-1}$, 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 ($J\cdot mol^{-1}\cdot K^{-1}$)		Group coefficients[a] C_i	
primary sp^3	CH_3–	17.6	(*A*1)		
secondary sp^3	$>CH_2$	7.1	(*A*2)	1.31[b]	(*B*2)
tertiary sp^3	–CH<	−16.4	(*A*3)	0.60	(*B*3)
quaternary sp^3	>C<	−34.8	(*A*4)	0.66	(*B*4)
secondary sp^2	$=CH_2$	17.3	(*A*5)		
tertiary sp^2	=CH–	5.3	(*A*6)	0.75	(*B*6)
quaternary sp^2	=C(R)–	−10.7	(*A*7)		
tertiary sp	H–C≡	14.9	(*A*8)		
quaternary sp	–C≡	−2.8	(*A*9)		
aromatic tertiary sp^2	$=C_aH$–	7.4	(*A*10)		
quaternary aromatic sp^2 carbon adjacent to an sp^3 atom	$=C_a(R)$–	−9.6	(*A*11)		
peripheral quaternary aromatic sp^2 carbon adjacent to an sp^2 atom	$=C_a(R)$–	−7.5	(*A*12)		
internal quaternary aromatic sp^2 carbon adjacent to an sp^2 atom	$=C_a(R)$–	−0.7	(*A*13)		

[a]The alphanumeric terms, *A*1, *A*2, *B*2, ... are a device used to identify each group value in the estimations provided in Tables 7, 8, and 9.
[b]The 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) ($J\cdot mol^{-1}\cdot K^{-1}$)		Group coefficient C_i	
Ring equations for nonaromatic cyclic compounds					
$\Delta S_{ring}=[33.4(A14)]+[3.7(A15)][n-3]$; n = number of ring atoms					
Ring equation for nonaromatic polycyclic compounds					
$\Delta S_{ring}=[33.4(A14)]N+[3.7(A15)][R-3N]$; R = total number of ring atoms; N = number of rings					
cyclic tertiary sp^3	$>C_cH(R)$	−14.7	(*A*16)		
cyclic quaternary sp^3	$>C_c(R)_2$	−34.6	(*A*17)		
cyclic tertiary sp^2	$=C_cH$–	−1.6	(*A*18)	1.92	(*B*18)
cyclic quaternary sp^2	$=C_c(R)$–	−12.3	(*A*19)		
cyclic quaternary sp	$=C_c=$; $R-C_c\equiv$	−4.7	(*A*20)		

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	(*A*21)					
chlorine	R–Cl	10.8	(*A*22)	1.5 (*B*22)	1.5 (*C*22)	1.5 (*D*22)	1.5 (*E*22)	1.5 (*F*22)
fluorine on an sp^2 carbon	═CRF	19.5	(*A*23)					
fluorine on an aromatic carbon	═CF–	16.6	(*A*24)					
3-fluorines on an sp^3 carbon	CF_3–R	13.3	(*A*25)					
2-flurorines on an sp^3 carbon	R—CF_2–R	16.4	(*A*26)					
1-fluorine on an sp^3 carbon	R—CF–$(R)_2$	12.7	(*A*27)					
fluorine on a ring carbon	–CHF–	[17.5]	(*A*28)					
	–CF_2–	[17.5]	(*A*28)					
iodine	R–I	19.4	(*A*29)					
hydroxyl group	R–OH	1.7	(*A*30)	10.4 (*B*30)	9.7 (*C*30)	13.1 (*D*30)	12.1 (*E*30)	13.1 (*F*30)
phenol	═C–(OH)–	20.3	(*A*31)					
ether	R—O–R	4.71	(*A*32)					
peroxide, 1	R–O–O–R	[10.6]	(*A*33)					
aldehyde	R–CH(═O)	21.5	(*A*34)					
ketone	R–C(═O)–(R)	4.6	(*A*35)					
carboxylic acid	R–C(═O)OH	13.4	(*A*36)	1.21 (*B*36)	2.25 (*C*36)	2.25 (*D*36)	2.25 (*E*36)	2.25 (*F*36)
formate ester	R–OCH(═O)	[4.2]	(*A*37)					
ester	R–C(═O)O–R	7.7	(*A*38)					
anhydride	R–C(═O)OC(═O)–R	[10.0]	(*A*39)					
acyl chloride	R–C(═O)Cl	[25.8]	(*A*40)					
aromatic heterocyclic amine	═N–	[10.9]	(*A*41)					
acyclic sp^2 nitrogen	═N–	[−1.8]	(*A*42)					
tertiary amine	R–N(R_2)	−22.2	(*A*43)					
secondary amine	R–NH–R	−5.3	(*A*44)					
primary amine	R–NH_2	21.4	(*A*45)					
azide	R–N_3	[−32.5]	(*A*46)					
tertiary amine *N*-nitro	R_2–N–(NO_2)	5.39	(*A*47)					
aliphatic secondary amine *N*-nitro	R–NH–(NO_2)	[−4.59]	(*A*48)					
aromatic tertiary amine-*N*-nitro	R–NH–(NO_2)	[−41.7]	(*A*49)					
nitro group	R–NO_2	17.7	(*A*50)					
N-nitro	>N–(NO_2)	39.8	(*A*51)					
N-nitroso	>N–N═O	[28.6]	(*A*52)					
oxime	═N–OH	[13.6]	(*A*53)					
azoxy nitrogen	N═N(→O)–	[6.8]	(*A*54)					
nitrate ester	R–ONO_2	[24.4]	(*A*55)					
nitrile	R–C≡N	17.7	(*A*56)					
isocyanide	R–NC	[17.5]	(*A*57)					
isocyanate	R–N═C═O	[23.1]	(*A*58)					
tertiary amides	R–C(═O)NR_2	−11.2	(*A*59)					
secondary amides	R–C(═O)NH–R	1.5	(*A*60)					
primary amide	R–$CONH_2$	27.9	(*A*61)					
N,N-dialkylformamide, 1	HC(═O)NR_2	[6.9]	(*A*62)					
tetra substituted urea	R_2NC(═O)NR_2	[−19.3]	(*A*63)					
1,1,3-trisubst urea	R_2NC(═O)NH–R	[0.2]	(*A*64)	−12.8 (*B*64)	−24 (*C*64)	6 (*D*64)		
1,1-disubstituted urea	R_2NC(═O)NH_2	[19.5]	(*A*65)					
1,3-disubstituted urea	RNHC(═O)NH–R	[1.5]	(*A*66)					
mono substituted urea	R–NHC(═O)NH_2	[22.5]	(*A*67)					
N,N-disubstituted carbamate	R–OC(═O)NR_2	−23.12	(*A*68)					
N-substituted carbamate	R–OC(═O)NH–R	10.6	(*A*69)					
carbamate	R–OC(═O)NH_2	[27.9]	(*A*70)					
imide	R–C(═O)NHC(═O)–R	[7.7]	(*A*71)					
phosphine	R_3–P	[−20.7]	(*A*72)					
phosphine oxide	R_3–P═O	[−32.7]	(*A*73)					
phosphate ester	P(═O)(O–$R)_4$	[−10.0]	(*A*74)					
phosphonate ester	R–P(═O)(O–$R)_2$	[−14.0]	(*A*75)					
phosphonic acid	R–P═O$(OH)_2$	[7.7]	(*A*76)					
phosphonyl halide	R–P(═O)X_2	[4.8]	(*A*77)					

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] k				
				2	3	4	5	6
phosphoramidate ester	$(R-O)_2P(=O)NH-R$	[−0.7]	(*A*78)					
phosphorothioate ester	$(R-O)_3P(=S)$	1.1	(*A*79)					
phosphorodithioate ester	$R-S-P(=S)(O-R)_2$	−9.6	(*A*80)					
phosphonothioate ester	$R-P(=S)(O-R)_2$	[5.2]	(*A*81)					
phosphoroamidothioate ester	$R-NHP(=S)(O-R)_2$	[16.0]	(*A*82)					
phosphoroamidodithioate ester	$NH_2P(=S)(S-R)(O-R)$	[6.9]	(*A*83)					
sulfides	R–S–R	2.1	(*A*84)					
disulfides	R–SS–R	9.6	(*A*85)					
thiols	R–SH	23.0	(*A*86)					
sulfoxide	$R-S(\rightarrow O)-R$	[14.1]	(*A*87)					
sulfones	$R-S(\rightarrow O)_2-R$	0.3	A88)					
sulfonate ester	$R-S(\rightarrow O)_2O-R$	[7.9]	(*A*89)					
1,2-disubstituted thiourea	$R-NHC(=S)NH-R$	[14.4]	(*A*90)					
monosubst thiourea	$R-NHC(=S)+NH_2$	[23.1]	(*A*91)					
thioamide	$R-C(=S)NH_2$	[30.0]	(*A*92)					
N,N disubstituted thiocarbamate	$R-S(C=O)N-R_2$	[5.6]	(*A*93)					
N,N-disubstituted sulfonamide	$R-S(\rightarrow O)_2N-R_2$,	[−11.3]	(*A*94)					
N-substituted sulfonamide	$R-S(\rightarrow O)_2NH-R$	6.3	(*A*95)					
sulfonic acid	$R-S(\rightarrow O)_2OH$	[1.8]	(*A*145)					
sulfonamide	$R-S(\rightarrow O)_2NH_2$	[28.4]	(*A*96)					
trisubstituted aluminum	R_3-Al	[−24.7]	(*A*97)					
trisubstituted arsenic	R_3-As	[−6.5]	(*A*98)					
trisubstituted boron	R_3-B	[−17.2]	(*A*99)					
trisubstituted bismuth	R_3-Bi	[−14.5]	(*A*100)					
trisubstituted galium	R_3-Ga	[−11.9]	(*A*101)					
tetrasubstituted germanium	R_4-Ge	[−35.2]	(*A*102)					
disubstituted germanium	R_2GeH_2	[−14.7]	(*A*103)					
disubstituted mercury	R_2-Hg	[8.4]	(*A*104)					
trisubstituted indium	R_3-In	[−19.3]	(*A*105)					
tetrasubstituted lead	R_4-Pb	[−30.2]	(*A*106)					
trisubstituted antimony	R_3-Sb	[−12.7]	(*A*107)					
disubstituted selenium	R_2-Se	[6.0]	(*A*108)					
quaternary silicon	R_4-Si	−27.1	(*A*109)					
quaternary tin	R_4-Sn	−24.2	(*A*110)					
disubstituted zinc	R_2-Zn	[11.1]	(*A*111)					
disubstituted telluride	R_2-Te	[−2.2]	(*A*140)					
trisubstituted germanium	R_3-GeH	[−27.8]	(*A*141)					
disubstituted arsinic acid	R_2-AsO_2H	[−24]	(*A*142)					
trisubstituted thallium	R_3-Th	[1]	(*A*143)					
disubstituted cadmium	R_2-Cd	[−2]	(*A*144)					

[a]R: any alkyl or aryl group unless specified otherwise; X: any halogen; units: J mol^{-1} K^{-1}.

[b]Unassigned 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	(*A*112)
cyclic peroxide	*R*–OO–*R*	[27.7]	(*A*113)
cyclic ketone	*R*–*C*(=*O*)–*R*	−1.4	(*A*114)
cyclic ester	*R*–*C*(=*O*)*O*–*R*	3.1	(*A*115)
cyclic carbonate	*R*–*OC*(=*O*)*O*–*R*	[1.3]	(*A*116)
cyclic anhydride	*R*–*C*(=*O*)–*O*–*C*(=*O*)–*R*	2.3	(*A*117)
cyclic sp^2 nitrogen	*R*=N–*R*	0.5	(*A*118)
cyclic tertiary amine	R_2>N–R	−19.3	(*A*119)
cyclic tertiary amine-N-nitro,	R_2>N–(NO_2)–R	−27.1	(*A*120)
cyclic tertiary amine-N-nitroso	R_2>N–(N=O)–R	−27.1	(*A*120)
cyclic secondary amine	R_2>NH	2.2	(*A*121)
cyclic tertiary amine N-oxide	R_2>N(→O)–R	[−22.2]	(*A*122)
cyclic azoxy group	*R*=N(→O)–*R*	[2.9]	(*A*123)
cyclic sec amide	*R*–C(=O)NH–*R*	2.7	(*A*124)
cyclic tertiary amide	*R*–C(=O)N<R*R*	−21.7	(*A*125)
cyclic tertiary amide	R–C(=*O*)*N*<R_2	[−9]	(*A*146)
cyclic carbamate	*R*–OC(=O)N–R*R*	[−5.2]	(*A*126)
cyclic carbamate	*R*–OC(=O)N–H*R*	[19.7]	(*A*125)
cyclic urea	*R*–NC(=O)N<R*R*	[−40.6]	(*A*127)
N-substituted cyclic imide	*R*–C(=O)N(R)C(=O)–*R*	[1.1]	(*A*128)
cyclic imide	*R*–C(=O)N(H)C(=O)–*R*	[1.4]	(*A*129)
cyclic phosphorothioate	*R*–O–P(=S)<(OR)(O*R*)	[−15.6]	(*A*130)
cyclic sulfide	*R*–S–*R*	2.9	(*A*131)
cyclic disulfide	*R*–SS–*R*	[−6.4]	(*A*132)
cyclic disulfide S-oxide	*R*–SS(→O)–*R*	[1.9]	(*A*133)
cyclic sulphone	*R*–S(→O)$_2$–*R*	[−10.4]	(*A*134)
cyclic thiocarbonate	*R*–OC(=O)S–*R*	[14.2]	(*A*135)
cyclic sulfate	*R*–OS(→O)$_2$O–*R*	0.9	(*A*136)
cyclic N-substituted sulphonamide	*R*–S(→O)$_2$NH–*R*	[−0.4]	(*A*137)
cyclic thiocarbamate	*R*–S–(C=O)NH*R*	[13.9]	(*A*138)
cyclic quaternary silicon	R_2>Si<R_2	−34.7	(*A*139)

[a]R: any alkyl or aryl group unless specified otherwise; values in brackets are tentative assignments; units: J mol^{-1} K^{-1}.
[b]The *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]

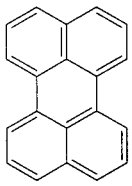
C_8H_8 styrene[b]

T_{fus}: 242.3 K
$\Delta_0^{T_{fus}}S_{tpce}$: 52.2 (45.2)
$\Delta_0^{T_{fus}}H_{tpce}$: 12.6 (11.0)
$\Delta_0^{T_{fus}}S_{tpce}$: {5[7.4]+[-7.5] +[5.3]+[17.3]}

C_7H_{14} 1-heptene[b]

T_{fus}: 154.3 K
$\Delta_0^{T_{fus}}S_{tpce}$: 77.5 (81.)
$\Delta_0^{T_{fus}}H_{tpce}$: 12.0 (12.6)
$\Delta_0^{T_{fus}}S_{tpce}$: {[17.3]+[5.3]+ 4[1.31][7.1]+17.6}

$C_{20}H_{12}$ perylene[b]

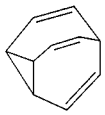


T_{fus}: 551 K
$\Delta_0^{T_{fus}}S_{tpce}$: 42.4 (57.9)
$\Delta_0^{T_{fus}}H_{tpce}$: 23.4 (31.9)
$\Delta_0^{T_{fus}}S_{tpce}$: {12[7.4]+ 6[-7.5]+2[-0.7]}

$C_{20}H_{32}$ 10,10,13,13-tetramethyl-1,5-cyclohexadecadiyne[c]

T_{fus}: 323 K
$\Delta_0^{T_{fus}}S_{tpce}$: 63.8 (58.3)
$\Delta_0^{T_{fus}}H_{tpce}$ 20.6 (18.8)
$\Delta_0^{T_{fus}}S_{tpce}$: {[33.4]+13[3.7] +4[17.6]+2[-34.6] 4[-4.7]}

$C_{10}H_{10}$ bullvalene[b]



T_{fus}: 366.5 K
$\Delta_0^{T_{fus}}S_{tpce}$: 35.3 (41.6)
$\Delta_0^{T_{fus}}H_{tpce}$: 12.9 (15.3)
$\Delta_0^{T_{fus}}S_{tpce}$: {3[33.4]+[3.7] 6[-1.6]+ 4[-14.7]}

$C_{12}H_8$ acenaphthylene[b,d]

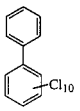
T_t: 116.6; 127.1 K
T_{fus}: 362.6 K
$\Delta_0^{T_{fus}}S_{tpce}$: 37.6 (12.1+19.1)
$\Delta_0^{T_{fus}}H_{tpce}$: 13.6 (1.5+6.9)
$\Delta_0^{T_{fus}}S_{tpce}$: {[33.4]+2[3.7] +[-7.5]+6[7.4] +3[-12.3]+2[-1.6]}

[a]Units for $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ 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).
[b]Reference 11.
[c]Reference 12.
[d]Reference 13.

TABLE 4. Estimations of total phase change entropies and enthalpies

A. Substituted Aromatic and Aliphatic Molecules[a]

$C_{12}Cl_{10}$ decachlorobiphenyl[b]



T_{fus}: 577.7 K
$\Delta_0^{T_{fus}}S_{tpce}$: 72.1 (68.1)
$\Delta_0^{T_{fus}}H_{tpce}$: 41.6 (39.3)
$\Delta_0^{T_{fus}}S_{tpce}$: {12[-7.5]+ {10[1.5][10.8]}

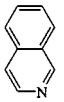
$C_5H_{10}N_2O_2$ N-acetyl-L-alanine amide[c]

T_{fus}: 431 K
$\Delta_0^{T_{fus}}S_{tpce}$: 54.9 (50.4)
$\Delta_0^{T_{fus}}H_{tpce}$: 23.7 (21.7)
$\Delta_0^{T_{fus}}S_{tpce}$: {2[17.6]+ [27.9]+0.6[-16.4]+[1.5]}

C_2F_3N 2,2,2-trifluoroacetonitrile[c]

T_{fus}: 128.7 K
$\Delta_0^{T_{fus}}S_{tpce}$: 34.6 (38.6)
$\Delta_0^{T_{fus}}H_{tpce}$: 4.5 (5.0)
$\Delta_0^{T_{fus}}S_{tpce}$: {[-34.8][0.66] 3[13.3]+[17.7]}

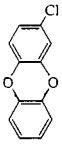
C_9H_7N isoquinoline[c]



T_{fus}: 299.6 K
$\Delta_0^{T_{fus}}S_{tpce}$: 47.9 (52.1)
$\Delta_0^{T_{fus}}H_{tpce}$: 14.3 (13.5)
$\Delta_0^{T_{fus}}S_{tpce}$: {[10.9]+7[7.4]+ 2[-7.5]}

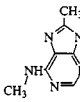
B. Substituted Cyclic Molecules[a]

$C_{12}H_7ClO_2$ 2-chlorodibenzodioxin[d]



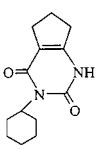
T_{fus}: 362.2 K
$\Delta_0^{T_{fus}}S_{tpce}$: 58.5 (63.8)
$\Delta_0^{T_{fus}}H_{tpce}$: 21.2 (23.1)
$\Delta_0^{T_{fus}}S_{tpce}$: {[33.4]+3[3.7] +2[1.2]+4[-12.3]+7[7.4]+ [-7.5]+[1.5][10.8]}

$C_8H_{11}N_5$ 6,8,9-trimethyladenine[e]



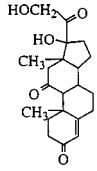
T_{fus}: 438 K
$\Delta_0^{T_{fus}}S_{tpce}$: 54.3 (52.7)
$\Delta_0^{T_{fus}}H_{tpce}$: 23.8 (23.1)
$\Delta_0^{T_{fus}}S_{tpce}$: {[33.4]+2[3.7] 3[17.6]+2[10.9]+[0.5]+ [-19.3]+[-5.3]+[-7.5]+ [7.4]+3[-12.3]}

$C_{13}H_{18}N_2O_2$ Lenacil[g]



T_{fus}: 584.3 K
$\Delta_0^{T_{fus}}S_{tpce}$: 64.0(72.4)
$\Delta_0^{T_{fus}}H_{tpce}$: 37.4 (42.3)
$\Delta_0^{T_{fus}}S_{tpce}$: {3[33.4] + 6[3.7]+2[-12.3]+ [-14.7]+[-21.7] [2.7]}

$C_{21}H_{28}O_5$ cortisone[f]



T_{fus}: 495 K
$\Delta_0^{T_{fus}}S_{tpce}$: 75.2 (74.5)
$\Delta_0^{T_{fus}}H_{tpce}$: 37.2 (36.9)
$\Delta_0^{T_{fus}}S_{tpce}$: {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]}

[a]Units for $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ are $J\cdot mol^{-1}\cdot K^{-1}$ and $kJ\cdot mol^{-1}$, respectively; experimental values are given in parentheses.
[b]Reference 14.
[c]Reference 11.
[d]Reference 15.
[e]Reference 16.
[f]Reference 17.
[g]Reference 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	11.6
		$A4*B4+A21+3*A22*D22$					[291]
CBr_4		carbon tetrabromide					
	320	5.94	18.58				
	363.2	3.95	10.88	29.46	47.3	9.9	17.2
		$A4*B4+4*A21$					[216]
CCl_3F		fluorotrichloromethane					
	162.7	6.9	0	42.38	38.4	6.9	6.2
		$A4*B4+3*A22*D22+A27$					[216]
CCl_4		carbon tetrachloride					
	224.6	4.6	20.49				
	249	2.69	10.82	31.31	41.9	7.3	10.4
	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	
		$4*A22*D22+A4*B4$					[216]
CF_4		carbon tetrafluoride					
	76.27	1.71	22.43				
	89.56	0.71	7.95	30.38	30.1	2.42	2.7
	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	
		$4*A25+A4*B4$					[216]
$CHClF_2$		chlorodifluoromethane					
	59	0.07	1.13				
	115.7	4.12	35.65	36.78	39.3	4.19	4.5
		$2*A26+A3*B3+A22*B22$					[216]
$CHCl_3$		trichloromethane					
	209.6	8.8	0	41.98	38.9	8.8	8.2
		$A3*B3+3*A22*C22$					[215]
CHF_3		trifluoromethane					
	118.0	4.06	0	34.85	30.5	4.06	3.6
		$3*A25+A3*B3$					[216]
CHF_3S		trifluoromethanethiol					
	116.0	4.93	0	42.44	39.9	4.93	4.6
		$3*A25+A4*B4+A86$					[216]
CH_2Cl_2		dichloromethane					
	178.2	6.16	0	34.56	39.5	6.16	7.0
		$A2+2*A22*B22$					[216]
CH_2N_2		cyanamide					
	317.2	8.76	0	27.62	39.1	8.76	12.4
	318.7	7.27	0	22.8		7.27	
		$A56+A45$					[215,216]
CH_2N_4		tetrazole					
	432.1	17.7	0	40.96	41.5	17.7	17.9
	430.7	18.4	0	42.7		18.4	
	242.5	0.014	0.06				
	430	18.0	41.9	42.0		18.14	
		$A14+2*A15+A121+3*A118+A18*B18$					[174,216]
CH_3Br		bromomethane					
	173.8	0.47	2.72				
	179.5	5.98	3.33	36.02	35.1	6.45	6.3
		$A21+A1$					[216]
CH_3Cl		methyl chloride					
	174.5	6.43	0	36.82	28.4	6.42	5.0
		$A1+A22$					[216]
CH_3ClFOP		methylphosphonyl chlorofluoride					
	250.7	11.85	0	47.28	51.2	11.85	12.8
		$A1+A22*C22+A27+A77$					[94]

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)
CH_3Cl_2OP		methylphosphonyl dichloride					
	306.1	18.08	0	59.05	54.8	18.08	16.8
		$A1+2*A22*C22+A77$					[94]
CH_3Cl_3Si		trichloromethylsilane					
	197.4	8.95	0	45.32	39.1	8.95	7.7
		$3*A22*D22+A1+A109$					[216]
CH_3F_2OP		methylphosphonyl difluoride					
	236.3	11.88	0	50.27	55.1	11.8	13.0
		$A1+2*A26+A77$					[94]
CH_3NO		formamide					
	275.7	7.98	0	28.94	27.9	7.98	7.7
	275.6	8.67	0	31.5		8.67	
		$A61$					[216]
CH_3NO_2		nitromethane					
	244.8	9.7	0	39.62	35.3	9.7	8.64
		$A1+A50$					[216]
CH_3NO_3		methyl nitrate					
	190.2	8.24	0	43.33	42.0	8.24	8.0
		$A1+A55$					[216]
CH_4O		methanol					
	161.1	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]
$CH_4N_4O_4$		N,N′-dinitro-diaminomethane					
	371	35.85	0	96.63	77.5	35.85	28.7
		$A2+2*A51+2*A48$					[225]
CH_4S		methanethiol					
	137.6	2.2	1.59				
	150.2	5.9	39.33	40.92	40.6	8.1	6.1
		$A1+A86$					[216]
CH_5N		methylamine					
	179.7	6.13	0	34.14	38.9	6.13	7.0
		$A1+A45$					[216]
CH_6N_2		methylhydrazine					
	220.8	10.42	0	47.19	33.7	10.42	7.4
		$A1+A44+A45$					[216]
$C_2Br_2F_2$		dibromodifluoroethylene					
	162.8	7.04	0	43.22	52.6	7.04	8.6
		$2*A21+2*A23+2*A7$					[216]
$C_2Br_2F_4$		1,2-dibromotetrafluoroethane					
	162.8	7.04	0	43.24	54.9	7.04	8.9
		$2*A4*B4+2*A21+4*A26$					[215]
C_2ClF_3		chlorotrifluoroethylene					
	115	5.55	0	48.28	53.2	5.55	6.1
		$2*A7+3*A23+A22*B22$					[216]
C_2ClF_5		pentafluorochloroethane					
	80.24	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]
$C_2Cl_2F_4$		1,2-dichloro-tetrafluoroethane					
	109.3	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]
$C_2Cl_3F_3$		1,1,2-trifluoro-1,2,2-trichloroethane					
	82.5	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_2Cl_4		tetrachloroethene					
	210	0.82	3.9				
	250.8	10.88	43.38	47.28	43.3	11.7	10.9
		$4*A22*D22+2*A7$					[216]
$C_2Cl_4F_2$		1,1,2,2-tetrachlorodifluoroethane					
	130	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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
		4*A22*E22+2*A27+2*A4*B4					[215,158]
C_2N_2		cyanogen					
	245.3	8.11	0	33.05	35.5	8.11	8.7
		2*A56					[216]
C_2Cl_6		hexachloroethane					
	318	2.57	8.07				
	345	8.22	23.83				
	458	9.75	21.29	53.18	51.4	20.54	23.5
		6*A22*F22+2*A4*B4					[216]
C_2F_3N		trifluoroacetonitrile					
	128.7	4.97	0	38.62	34.6	4.97	4.5
		3*A25+A4*B4+A56					[216]
C_2F_4		tetrafluoroethylene					
	142	7.71	0	54.31	56.5	7.71	8.0
		4*A23+2*A7					[216]
C_2F_6		hexafluoroethane					
	104.0	3.74	35.9				
	173.1	2.69	15.5	51.4	33.8	6.0	6.0
		6*A25+2*A4*B4					[216]
$C_2HBrClF_3$		2-bromo-2-chloro-1,1,1-trifluoroethane					
	154.7	4.84	0	31.29	41.0	4.84	6.3
		A22*C22+A21+3*A25+A4*B4+A3*B3					[216]
$C_2HBrClF_3$		1-bromo-2-chloro-1,1,2-trifluoroethane					
	146.2	4.38	0	29.96	46.6	4.38	6.8
		A22*C22+A21+2*A26+A4*B4+A3*B3+A27					[216]
C_2HCl_3		trichloroethylene					
	188.5	8.45	0	44.83	41.8	8.45	7.9
		3*A22*C22+A6*B6+A7					[216]
$C_2HCl_3O_2$		trichloroacetic acid					
	330.7	5.88	0	17.78	55.7	5.88	18.4
		3*A22*D22+A36*D36+A4*B4					[215]
$C_2H_2Br_2F_2$		1,2-dibromo-1,1-difluoroethane					
	206.3	8.3	0	40.23	52.1	8.3	10.8
		2*A21+2*A26+A2+A4*B4					[215]
$C_2H_2Cl_2$		1,1-dichloroethene					
	150.9	6.51	0	43.26	39.0	6.51	5.9
		2*B22*A22+A7+A5					[216]
$C_2H_2Cl_2F_2$		1,2-difluoro-2,2-dichloroethane					
	163.0	8.19	0	50.26	42.0	8.19	6.8
		2*A22*C22+A4*B4+2*A27+A2					[216]
$C_2H_2Cl_2O_2$		dichloroacetic acid					
	286.5	12.34	0	43.08	52.8	12.34	15.1
		2*A22*C22+A3*B3+A36*C36					[216]
$C_2H_2Cl_4$		1,1,2,2-tetrachloroethane					
	207.3	0.54	2.62				
	230.8	9.17	39.74	42.38	45.4	9.72	10.5
	204.8	0.36	1.74				
	230.3	9.52	41.5	43.2		9.88	
		2*A3*B3+4*A22*D22					[216]
$C_2H_3Br_3$		1,1,2-tribromoethane					
	244	9.11	0	37.34	50.1	9.11	12.2
		A2+A3*B3+3*A21					[215]
C_2H_3Cl		vinyl chloride					
	119.3	4.92	0	41.21	32.0	4.92	3.8
		A5+A6*B6+A22					[216]
$C_2H_3ClF_2$		1,1-difluoro-1-chloroethane					
	142.4	2.69	0	18.86	43.6	2.69	6.2
		2*A26+A22*B22+A1+A4*B4					[216]
$C_2H_3ClO_2$		(α form) chloroacetic acid					
	334.3	16.3	0	48.74	39.4	16.3	13.2
		A22*B22+A2+A36*B36					[216]
$C_2H_3ClO_2$		(β form) chloroacetic acid					
	329.2	13.93	0	42.33	39.4	13.93	13.0
		A22*B22+A2+A36*B36					[216]
$C_2H_3Cl_3$		1,1,2-trichloroethane					
	237.1	11.38	0	48	46.0	11.38	10.9
	237.9	10.9	0	45.7		10.9	
		3*A22*C22+A2+A3*B3					[74]
$C_2H_3Cl_3$		1,1,1-trichloroethane					

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)
	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	
		3*A22*C22+A4*B4+A1					[216]
$C_2H_3F_3$		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	
		3*A25+A4*B4+A1					[215]
C_2H_3N		acetonitile					
	216.9	0.9	4.14				
	229.3	8.17	35.61	39.75	35.3	9.06	8.1
		A1+A56					[216]
$C_2H_3N_3$		1,2,4-triazole					
	393.5	16.1	0	40.91	37.8	16.1	14.9
		A14+2*A15+2*A118+A121+2*A18*B18					[216]
C_4H_4		ethylene					
	104.0	3.35	0	32.24	34.7	3.35	3.6
		2*A5					[216]
C_2H_4BrCl		1-bromo-2-chloroethane					
	182	3.1	17.15				
	256.4	9.62	37.53	54.69	48.0	12.72	12.3
		2*A2+A21+A22*B22					[216]
$C_2H_4Br_2$		1,2-dibromoethane					
	249.5	1.94	7.78				
	283	10.94	38.66	46.44	49.4	12.88	14.0
		2*A21+2*A2					[216]
$C_2H_4Cl_2$		1,1-dichloroethane					
	176.2	7.87	0	44.77	40.3	7.87	7.1
		2*B22*A22+A1+A3*B3					[215]
$C_2H_4Cl_2$		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	
		2*A22*B22+2*A2					[216]
$C_2H_4D_2O_2$		dihydroxyethane-d_2					
	258.8	9.75	0	37.67	50.5	9.75	13.1
		2*A2+2*A30*B30					[55]
$C_2H_4N_4$		1H-1,2,4-triazol-3-amine					
	428.3	21.93	0	51.2	52.2	21.93	22.4
		A14+2*A15+2*A121+2*A118+A18*B18+A19+A45					[221]
$C_2H_4N_4$		1-methyltetrazole					
	315	15.7	0	49.85	37.5	15.7	11.8
		A14+2*A15+A119+3*A118+A1+A18*B18					[174]
$C_2H_4N_4$		2-methyltetrazole					
	286	12.37	0	43.25	37.5	12.37	10.7
		A14+2*A15+A119+3*A118+A1+A18*B18					[174]
$C_2H_4N_4$		5-methyltetazole					
	418	16	0	38.28	49.9	16	20.8
		A14+2*A15+3*A118+A121+A1+A19					[174]
C_2H_4O		ethylene oxide					
	160.7	5.17	0	32.22	34.6	5.17	5.6
		A14+A112					[216]
C_2H_4O		acetaldehyde					
	149.8	2.31	15.42				
	242.9	1.72	7.06	22.49	39.1	4.03	9.5
		A1+A34					[216]
$C_2H_4O_2$		ethanoic acid					
	298.7	11.72	0	39.24	31.0	11.72	9.2
		A36+A1					[216]
C_2H_5Cl		chloroethane					
	134.8	4.45	0	33.01	35.5	4.45	4.8
		A22+A2+A1					[215]
$C_2H_5Cl_3Si$		ethyltrichlorosilane					
	165.3	6.96	0	42.1	46.2	6.96	7.6
		A1+A2+3*A22*C22+A109					[216]
C_2H_5NO		acetamide					

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	353	15.6	0	44.19	45.5	15.6	16.1
	354	15.5	0	43.8		15.5	
		*A*1+*A*61					[271,216]
$C_2H_5NO_2$		nitroethane					
	183.7	9.85	0	53.64	42.4	9.85	7.8
		*A*1+*A*2+*A*50					[216]
$C_2H_5NO_2$		methyl carbamate					
	328.6	16.7	0	50.82	45.5	16.7	14.9
		*A*1+*A*70					[216]
$C_2H_5NO_3$		ethyl nitrate					
	178.6	8.53	0	47.74	49.1	8.53	8.8
		*A*1+*A*2+*A*55					[126]
C_2H_5NS		ethanethioamide					
	385.7	18.36	0	47.59	47.6	18.36	18.4
		*A*1+*A*92					[221]
C_2H_6		ethane					
	89.5	2.79	0	31.21	35.2	2.79	3.2
	89.9	2.86	0	31.8		2.86	
		2**A*1					[216]
$C_2H_6ClO_3P$		2-chloroethylphosphonic acid					
	347.9	14.79	0	42.51	42.6	14.79	14.8
		2**A*2+*A*22**B*22+*A*76					[221]
$C_2H_6Cl_2Si$		dimethyldichlorosilane					
	199.0	8.83	0	44.36	40.5	8.83	8.1
		2**A*1+2**A*22**C*22+*A*109					[216]
$C_2H_6N_2O$		N-methylurea					
	378.1	14.06	0	37.19	40.09	14.06	15.16
	373.8	15.75		42.1		15.75	
		*A*1+*A*67					[138,216]
$C_2H_6N_2O_2$		N-nitro-N-methylaminomethane					
	327	37.66	0	115.16	80.3	37.66	26.3
		2**A*1+*A*51+*A*47					[225]
$C_2H_6N_4O_4$		N,N′-dinitroethanediamine					
	450	29.5	0	65.55	84.6	29.5	38.07
		2**A*2+2**A*48+2**A*51					[225]
C_2H_6O		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	
		*A*1+*A*2+*A*30					[216]
C_2H_6O		dimethyl ether					
	131.7	4.94	0	37.5	39.9	4.94	5.3
		2**A*1+*A*32					[216]
C_2H_6OS		dimethyl sulfoxide					
	291.7	14.37	0	49.26	49.3	14.37	14.4
		2**A*1+*A*87					[216]
$C_2H_6O_2$		dihydroxyethane					
	260.6	9.96	0	38.21	50.5	9.96	13.2
	260.8	11.6	0	44.6		11.6	
		2**A*2+2**A*30**B*30					[216]
$C_2H_6O_2S$		dimethylsulfone					
	382	18.28	0	47.91	35.4	18.30	13.5
		2**A*1+*A*88					[216]
C_2H_6S		ethyl mercaptan					
	195.3	4.97	0	25.48	47.7	4.97	9.3
		*A*1+*A*2+*A*86					[216]
C_2H_6S		dimethyl sulfide					
	174.9	7.98	0	45.66	37.3	7.98	6.5
		2**A*1+*A*84					[216]
$C_2H_6S_2$		dimethyldisulfide					
	188.4	9.19	0	48.78	44.7	9.19	8.4
		2**A*1+*A*85					[216]
C_2H_6Se		dimethylselenium					
	185.1	8.5	0	45.91	41.1	8.5	7.6
		2**A*1+*A*108					[170]
$C_2H_6Se_2$		dimethyldiselenium					
	190.8	8.55	0	44.78	47.1	8.55	9.0
		2**A*1+2**A*108					[170]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
C_2H_6Zn		dimethyl zinc					
	210.3	1.06	5.05				
	230.1	6.83	29.68	34.73	46.2	7.89	10.6
		2*A1+A111					[216]
$C_2H_7AsO_2$		hydroxydimethyl arsine					
	470.9	24.46	0	51.93	46.8	24.46	22.0
		2*A1+A98+A30*B30					[221]
C_2H_7N		dimethyl amine					
	181.0	5.94	0	29.68	29.9	5.94	5.4
		2*A1+A44					[216]
$C_2H_8NOPS_2$		O,S-dimethyl phosphoroamidothioate					
	316.8	13.34	0	42.1	42.1	13.34	13.3
		2*A1+A83					[221]
$C_2H_8N_2$		diaminoethane					
	189.0	0.49	2.57				
	284.2	22.58	79.43	82.05	57.0	23.07	16.2
		2*A45+2*A2					[201]
$C_2H_8N_2$		N,N-dimethylhydrazine					
	216.0	10.07	0	46.64	34.3	10.07	7.4
		2*A1+A45+A43					[216]
$C_2H_8N_2$		N,N′-dimethylhydrazine					
	264.3	13.64	0	51.6	24.6	13.64	6.5
		2*A1+2*A44					[216]
C_3Cl_6		hexachlorocyclopropane					
	376	18.6	49.47	49.47	26.8	18.6	10.1
		6*A22*F22+3*A17+A14					[216]
C_3F_6O		hexafluoroacetone					
	147.7	8.38	0	56.74	38.3	8.38	5.7
		6*A25+2*A4*B4+A35					[216]
C_3F_8		octafluoropropane					
	99.4	3.56	35.77				
	125.5	0.48	3.81	39.58	43.6	4.03	5.5
		2*A26+3*A4*B4+6*A25					[216]
$C_3H_2ClF_5$		3-chloro-1,1,1,3,3-pentafluoropropane					
	165.4	10.47	0	63.3	50.07	10.47	8.28
		2*A26+A22*B22+2*A4*B4+A2+3*A25					[216]
$C_3H_2Cl_3F_3$		1,1,1-trichloro-3,3,3-trifluoropropane					
	232.7	14.07	0	60.46	49.71	14.07	11.57
		3*A22*D22+3*A25+A2+2*A4*B4					[215]
$C_3H_2N_2$		dicyanomethane					
	305.0	10.8	0	35.4	42.59	10.8	12.99
		2*A56+A2					[216]
$C_3H_3Cl_2F_3$		1,1,1-trifluoro-3,3-dichloropropane					
	167.7	0.2	1.21				
	182.2	10.13	55.65	56.86	46.7	10.33	8.5
		3*A25+A4*B4+A3*B3+A2+2*A22C22					[216]
C_3H_3N		acrylonitrile					
	162.5	1.19	7.32				
	189.6	6.23	32.84	40.17	39.0	7.42	7.4
		A5+B6*A6+A56					[216]
C_3H_3NS		thiazole					
	239.4	9.58	40.08	40.04	35.0	9.58	8.5
		A14+2*A15+A131+A118+3*A18*B18					[59,61]
$C_3H_3N_3$		*s*-triazine					
	197.7	0.07	0.37				
	353.4	14.56	41.2	41.57	55.0	14.63	19.4
		3*A10+3*A41					[215]
$C_3H_4ClF_3$		1,1,1-trifluoro-3-chloropropane					
	169.8	4.49	26.44				
	179.3	5.05	28.2	54.6	47.3	9.54	8.5
		3*A25+A4*B4+2*A2+A22*B22					[216]
$C_3H_4Cl_3NSi$		β-trichlorosilylpropionitrile					
	307.9	21.24	0	68.99	53.5	21.24	16.5
		2*A2+A56+3*A22*E22+A109					[103]
$C_3H_4Cl_4$		1,1,1,3-tetrachloropropane					
	219.9	2.2	10.03				
	237.7	10.49	44.13	54.16	56.2	12.69	13.4
		4*A22*D22+A4*B4+2*A2					[216]
$C_3H_4N_2$		imidazole					
	361.9	12.8	0	35.37	37.3	12.8	13.5

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)
		$A14+2*A15+2*A18*B18+A118+A121$					[216]
$C_3H_4N_2$		pyrazole					
	343.2	14.2	0	41.38	37.3	14.2	12.8
		$A14+2*A15+2*A18*B18+A118+A121$					[216]
$C_3H_4N_2O$		cyanoacetamide					
	346.5	1.2	3.46				
	387.3	21.7	56.03	59.49	52.8	22.9	20.4
		$A2+A56+A61*B61$					[216]
$C_3H_4O_2$		acrylic acid					
	285.5	11.16	0	39.09	34.6	11.16	9.9
		$A5+A6*B6+A36$					[215]
$C_3H_4O_2$		β-propiolactone					
	239.9	9.41	0	39.22	40.2	9.41	9.7
		$A14+A15+A115$					[32]
$C_3H_4O_3$		ethylene carbonate					
	309.5	13.3	0	42.96	42.1	13.3	13.0
		$A14+2*A15+A116$					[52]
$C_3H_5Br_3$		1,2,3-tribromopropane					
	289.4	23.78	0	82.17	57.3	23.78	16.6
		$2*A2+A3*B3+3*A21$					[215]
C_3H_5N		propionitrile					
	177.0	17.07	9.67				
	180.4	5.03	27.91	37.57	42.4	22.1	7.7
		$A1+A2+A56$					[216]
C_3H_5NO		acrylamide					
	358	15.33	0	42.82	49.2	15.33	17.6
		$A5+A6*B6+A61$					[216]
$C_3H_5N_3O_9$		trinitroglycerine					
	285.5	21.87	0	76.6	77.8	21.87	22.2
		$2*A2+A3*B3+3*A55$					[215]
C_3H_6		propene					
	88.2	2.93	0	33.3	40.2	2.93	3.5
	87.85	3.0		34.18		3.0	
		$A1+A5+A6$					[216]
C_3H_6		cyclopropane					
	145.6	5.44	0	37.4	33.4	5.44	4.9
		$A14$					[216]
$C_3H_6Br_2$		1,3-dibromopropane					
	238.6	14.64	0	61.5	63.1	14.64	15.1
		$2*A21+3*A2*B2$					[216]
$C_3H_6ClNO_2$		2-chloro-2-nitropropane					
	213.8	9.54	44.62				
	261.6	1.34	5.1	49.72	46.2	10.88	12.1
		$2*A1+A4*B4+A50+A22*B22$					[216]
$C_3H_6Cl_2$		1,2-dichloropropane					
	172.7	6.4	0	37.06	47.4	6.4	8.2
		$A1+A2+A3*B3+2*A22*B22$					[215]
$C_3H_6Cl_2$		2,2-dichloropropane					
	188	5.98	31.8				
	239.3	2.34	9.62	41.42	44.7	8.32	10.8
		$2*B22*A22+2*A1+A4*B4$					[216]
$C_3H_6N_2O_2$		malonamide					
	393	1.9	4.83				
	443	35.8	80.81	85.65	63.0	37.7	27.9
		$2*A61+A2$					[292]
$C_3H_6N_2O_4$		2,2-dinitropropane					
	267.7	11.28	42.13				
	259.7	1.87	7.2				
	324.5	2.64	8.12	57.15	47.8	15.78	15.5
		$2*A1+A4*B4+2*A50$					[216]
$C_3H_6N_4$		1,5-dimethyltetrazole					
	349	14.7	0	42.12	46.0	14.7	16.0
		$A14+2*A15+3*A118+A119+A19+2*A1$					[174]
$C_3H_6N_4$		2,5-dimethyltetrazole					
	256.4	13.5	0	52.65	46.0	13.5	11.8
		$A14+2*A15+3*A118+A119+A19+2*A1$					[174]
$C_3H_6N_4O_4$		1,3-dinitro-1,3-diazacyclopentane					
	410	25.1	0	62.3	66.2	25.1	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_3H_6N_6O_3$		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
		*A*14+3**A*15+3**A*120+3**A*52					[216]
$C_3H_6N_6O_5$		1,3-dinitro-5-nitroso-1,3,5-triazacyclohexane					
	446	25.97	0	58.24	71.4	25.97	31.8
		*A*14+*A*15*3+3**A*120+2**A*51+*A*52					[225]
$C_3H_6N_6O_6$		1,3,5-trinitro-1,3,5-triazacyclohexane					
	478.2	37.66	0	78.75	82.6	37.66	39.5
		*A*14+*A*15*3+3**A*120+3**A*51					[216]
C_3H_6O		acetone					
	176.6	5.72	0	32.34	39.7	5.72	7.0
		2**A*1+*A*35					[216]
C_3H_6O		propylene oxide					
	161.3	6.57	0	40.75	37.5	6.57	6.0
	161.2	6.53	0	40.52		6.53	
		*A*1+*A*14+*A*112+*A*16					[216]
C_3H_6O		propanal					
	171.3	8.59	0	50.14	46.3	8.59	7.9
		*A*1+*A*2+*A*34					[216]
$C_3H_6O_2$		propionic acid					
	252.7	10.66	0	42.2	38.1	10.66	9.6
		*A*1+*A*2+*A*36					[216]
$C_3H_6O_2$		1,3-dioxolane					
	142.4	2.68	18.8				
	175.9	6.57	37.33	56.13	43.2	9.24	7.6
		*A*14+2**A*15+2**A*112					[216]
$C_3H_6O_2$		methyl acetate					
	174.9	7.49	0	42.82	42.8	7.49	7.5
		2**A*1+*A*38					[1]
$C_3H_6O_2S$		β-thiolactic acid					
	291.9	16.97	0	58.15	53.4	16.97	15.6
		2**A*2+*A*36+*A*86					[216]
$C_3H_7O_3$		DL lactic acid					
	289.9	11.34	0	39.12	42.2	11.34	12.2
		*A*1+*A*3**B*3+*B*30**A*30+*A*36**B*36					[216]
$C_3H_6O_3$		1,3,5-trioxane					
	333.4	15.11	0	45.3	48.2	15.11	16.1
		*A*14+3**A*15+3**A*112					[215]
C_3H_6S		thiacyclobutane					
	176.7	0.67	3.77				
	199.9	8.24	41.25	45.02	40.0	8.91	8.0
		*A*14+*A*15+*A*131					[216]
C_3H_7Br		2-bromopropane					
	184.1	6.53	0	35.5	43.1	6.53	7.9
		2**A*1+*A*3**B*3+*A*21					[216]
C_3H_7Cl		2-chloropropane					
	156	7.39	0	47.37	36.3	7.39	5.7
		*A*3**B*3+2**A*1+*A*22					[215]
C_3H_7N		cyclopropylamine					
	237.8	13.18	0	55.44	40.0	13.18	9.5
		*A*14+*A*45+*A*16					[215]
C_3H_7NO		N,N-dimethylformamide					
	212.9	8.95	0	42.05	42.1	8.95	9.0
		2**A*1+*A*62					[216]
C_3H_7NO		N-methylacetamide					
	303.8	9.73	0	32.01	36.6	9.73	11.1
		2**A*1+*A*60					[270]
$C_3H_7NO_2$		ethyl carbamate					
	321.9	15.23	0	47.31	52.6	15.23	16.9
	321.7	20.9	0	64.8		20.9	
	321.4	16.8	0	52.3		16.8	
		*A*1+*A*2+*A*70					[215, 216]
$C_3H_7NO_3$		isopropyl nitrate					
	190.9	10.1	0	52.9	49.9	10.1	9.5
		2**A*1+*A*3**B*3+*A*55					[173]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
C_3H_8		propane					
	85.5	3.52	0	41.24	42.3	3.52	3.6
		2*A1+A2					[215]
$C_3H_8N_2O$		N-ethylurea					
	365.1	14.39	0	39.41	47.2	14.39	17.2
	367.8	13.9	0	37.9		13.9	
		A1+A2+A67					[138]
$C_3H_8N_2O$		1,1-dimethylurea					
	454	29.11	0	64.12	54.7	29.11	24.8
		2*A1+A65					[215]
$C_3H_8N_2O$		1,3-dimethylurea					
	379.5	13	34.26				
	301.2	0.08	0.26				
	161.3	0.32	1.97	36.48	36.6	13.4	5.91
		2*A1+A66					[124, 138]
C_3H_8O		1-propanol					
	148.8	5.37	0	36.12	33.6	5.37	5.0
		A1+2*A2+A30					[73]
C_3H_8O		2-propanol					
	185.2	5.41	0	29.21	27.3	5.41	5.1
	184.7	5.37	0	29.1		5.37	
		2*A1+A3*B3+A30					[216]
$C_3H_8O_2$		dimethoxymethane					
	168.0	8.33	0	49.59	51.7	8.33	8.7
		2*A1+A2+2*A32					[216]
$C_3H_8O_3$		1,2,3-trihydroxypropane					
	293	18.28	0	62.34	55.6	18.28	16.3
	291	18.28	0	62.8		18.28	
		2*A2+A3*B3+3*A30*C30					[215]
C_3H_8S		ethyl methyl sulfide					
	167.2	9.76	0	58.37	44.4	9.76	7.4
		2*A1+A2+A84					[216]
C_3H_8S		1-propanethiol					
	142.1	3.97	27.95				
	160	5.48	34.23	62.17	54.9	9.45	8.8
		A1+2*A2+A86					[216]
C_3H_8S		2-propanethiol					
	112.5	0.05	0.46				
	142.6	5.74	40.21	40.67	48.5	5.78	6.9
		2*A1+A3*B3+A86					[216]
$C_3H_8SO_2$		ethylmethylsulfone					
	307.7	11.3	0	36.71	42.6	11.3	13.1
		2*A1+A2+A88					[276]
C_3H_9Al		trimethylaluminum					
	288.4	8.79	0	30.48	28.1	8.79	8.1
		3*A1+A97					[216]
C_3H_9As		trimethylarsine					
	186.6	8.96	0	48.03	46.3	8.96	8.6
		3*A1+A98					[171]
C_3H_9B		trimethylborane					
	113.2	3.25	0	28.68	35.6	3.25	4.0
		3*A1+A99					[216]
C_3H_9ClSi		chlorotrimethylsilane					
	185.1	0.7	3.75				
	218.0	9.68	44.42	48.17	41.8	10.38	9.1
		3*A1+A22*B22+A109					[216]
C_3H_9Ga		trimethylgallium					
	257.9	11.05	0	42.83	40.8	11.05	10.5
	244.5	0.33	1.4				
	257.8	10.6	41.1	42.5		11.0	
		3*A1+A101					[216]
C_3H_9N		1-aminopropane					
	188.4	10.97	0	58.24	53.2	10.97	10.0
	188.4	10.63	0	56.4		10.63	
		A1+2*A2+A45					[215, 216]
C_3H_9N		2-aminopropane					
	178	7.33	0	41.17	46.9	7.33	8.3
		2*A1+A3*B3+A45					[215]
C_3H_9N		trimethylamine					
	156.1	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_{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)
$C_3H_{10}N_2$		1,2-diaminopropane					
	222	0.07	0.3				
	236.5	18.42	77.89	78.19	57.8	18.49	13.7
		*A*2+*A*3**B*3+*A*1+2**A*45					[50]
$C_3H_{10}N_2$		trimethylhydrazine					
	201.2	9.49	0	47.13	25.2	9.49	5.1
		3**A*1+*A*44**B*44+*A*43					[216]
$C_4H_2O_3$		maleic anhydride					
	325.7	12.26	0	37.65	36.9	12.26	12.0
		*A*14+2**A*15+2**A*18**B*18+*A*117					[216]
C_4H_3BrS		2-bromothiophene					
	55.3	0.01	0.25				
	205.3	7.9	38.43	38.7	42.7	7.91	8.7
		*A*14+2**A*15+*A*21+*A*131+2**A*18+*A*18**B*18+*A*19					[64]
C_4H_3ClS		2-chlorothiophene					
	201.3	8.97	0	44.56	41.3	8.97	8.3
		*A*14+2**A*15+*A*22**B*22+*A*131+2**A*18+*A*18**B*18+*A*19					[37]
$C_4H_3F_5O_3$		α-(trifluoromethoxy)-α,α-difluoromethyl acetate					
	167.4	8.51	0	50.84	52.0	8.51	8.7
		3**A*25+2**A*26+*A*1+*A*38+2**A*4**B*4					[216]
$C_4H_4N_2$		pyrazine					
	328.2	12.95	0	39.46	51.5	12.95	16.9
		4**A*10+2**A*41					[272]
$C_4H_4N_2$		succinonitrile					
	233.3	6.2	26.57				
	331.2	3.7	11.21	37.78	49.7	9.9	16.5
		2**A*56+2**A*2					[216]
$C_4H_4N_4O_2$		N-nitro-bis(N,N-cyanomethyl) amine					
	367	38.66	0	105.34	94.9	38.66	34.8
		2**A*2+2**A*56**C*56+*A*51**C*51+*A*47**C*47					[225]
C_4H_4O		furan					
	150.0	2.05	13.64				
	187.6	3.8	20.29	33.93	32.6	5.85	6.1
		*A*14+2**A*15+*A*112+2**A*18**B*18+2**A*18					[216]
$C_4H_4O_4$		1,4-dioxane-2,5-dione					
	312.1	1.81	5.82				
	356.2	14.8	41.55	47.36	50.8	16.61	18.1
		3**A*15+*A*14+2**A*115					[216]
$C_4H_4O_4$		ethylene oxalate					
	415	13.4	0	32.29	50.8	13.4	21.1
		*A*14+3**A*15+2**A*115					[216]
C_4H_4S		thiophene					
	171.1	1.21	7.11				
	233.7	4.97	21.34	28.45	34.3	6.18	8.1
	171.6	0.64	3.7				
	235.0	5.09	21.65	25.4		5.7	
		*A*14+2**A*15+2**A*18**B*18+*A*131+2**A*18					[216, 2]
$C_4H_5ClO_2$		*cis*-3-chloro-2-butenoic acid					
	333.7	13.81	0	41.42	43.1	13.81	14.4
		*A*36**B*36+*A*1+*A*7+*A*6**B*6+*B*22**A*22					[216]
$C_4H_5ClO_2$		Z-3-chloro-2-butenoic acid					
	366.8	20.71	0	56.48	43.09	20.71	15.81
		*A*36**B*36+*A*1+*A*6**B*6+*A*7+*A*22**B*22					[216]
$C_4H_5ClO_2$		E-3-chloro-2-butenoic acid					
	333.7	13.81	0	41.38	43.1	13.81	14.4
		*A*36**B*36+*A*1+*A*6**B*6+*A*7+*A*22**B*22					[216]
C_4H_5N		pyrrole					
	249.7	7.91	0	31.66	33.6	7.91	8.4
		2**A*18+*A*121+*A*14+2**A*15+2**A*18**B*18					[216]
$C_4H_5NO_2$		succinimide					
	400	17.0	0	42.5	42.2	17.0	16.9
		*A*14+2**A*15+*A*129					[216]
C_4H_5NS		2-methylthiazole					
	248.6	12.16	43.44	48.91	43.3	12.16	10.8
		*A*14+2**A*15+*A*131+*A*118+*A*1+2**A*18**B*18+*A*19					[57, 58]
C_4H_5NS		4-methylthiazole					
	229.1	8.9	0	38.85	43.3	8.9	9.9
		*A*14+2**A*15+*A*131+*A*118+*A*1+2**A*18**B*18+*A*19					[61]
C_4H_5NS		5-methylthiazole					

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)
	232.8	7.65	0	32.86	43.3	7.65	10.1
		$A14+2*A15+A131+A118+A1+2*A18*B18+A19$					[61]
C_4H_6		1,3-butadiene					
	164.2	7.98	0	48.62	45.2	7.98	7.4
		$2*A5+2*A6$					[215]
C_4H_6		1,2-butadiene					
	136.9	6.96	0	50.8	37.4	6.96	5.1
		$A1+A5+A9+A6$					[216]
C_4H_6		2-butyne					
	240.9	9.25	0	38.38	29.6	9.25	7.1
		$2*A1+2*A9$					[215]
C_4H_6		1-butyne					
	147.4	6.03	0	40.9	36.9	6.03	5.4
		$A1+A2+A9+A8$					[216]
$C_4H_6N_6O_8$		1,3,5,5-tetranitro-1,3-diazacyclohexane					
	430	29.37	0	68.31	70.8	29.37	30.4
		$A14+3*A15+2*A120+2*A51+2*A50+A17$					[225,193]
$C_4H_6O_2$		methyl acrylate					
	197.5	9.73	0	49.26	46.5	9.73	9.2
		$A1+A5+A6*B6+A38$					[216]
$C_4H_6O_2$		α-methylacrylic acid					
	287.5	8.06	0	28.04	37.6	8.06	10.8
		$A1+A36+A7+A5$					[216]
$C_4H_6O_2$		*cis*-crotonic acid					
	344.4	12.57	0	36.49	40.1	12.57	13.8
		$A1+A6+A36+A6*B6$					[215]
$C_4H_6O_2$		γ-butyrolactone					
	230	9.57	0	41.84	43.9	9.57	10.1
		$A14+2*A15+A115$					[32]
$C_4H_6O_3$		propylene carbonate					
	218.2	9.62	0	44.07	44.9	9.62	9.8
		$2*A15+A14+A1+A16*B16+A116$					[89]
$C_4H_6O_4$		dimethyl oxalate					
	327.6	21.07	0	64.32	50.5	21.07	16.5
		$2*A1+2*A38*B38$					[215]
$C_4H_6O_4$		succinic acid					
	457	32.95	0	72.1	46.5	32.95	21.3
		$2*A36*B36+2*A2$					[340]
$C_4H_6O_5$		(*dl*) malic acid I					
	402	33.52	0	83.39	74.5	33.52	30.0
		$A2+2*C36*A36+A3*B3+A30*C30$					[216]
$C_4H_6O_5$		(*dl*) malic acid II					
	396	30.17	0	76.19	74.5	30.17	29.5
		$A2+2*C36*A36+A3*B3+A30*C30$					[216]
$C_4H_6O_5$		(*d*) malic acid					
	376	23.01	0	61.2	74.5	23.01	28.0
		$A3*B3+2*C36*A36+A2+A30*C30$					[273]
C_4H_7NO		2-pyrrolidone					
	299	13.92	0	46.56	43.5	13.92	13.0
C_4H_7NO		$A14+2*A15+A124$					[216]
	385.1	methacrylamide					
		15	0	38.95	52.1	15	20.1
		$A1+A7+A5+A61$					[216]
C_4H_8		cyclobutane					
	145.7	5.71	39.17				
	182.4	1.09	5.96	45.13	37.1	6.79	6.8
		$A14+A15$					[216]
C_4H_8		1-butene					
	87.8	3.85	0	43.84	47.3	3.85	4.2
		$A1+A2+A5+A6$					[216]
C_4H_8		*cis*-2-butene					
	134.3	7.31	0	54.43	45.7	7.31	6.1
		$2*A1+2*A6$					[216]
C_4H_8		*trans*-2-butene					
	167.6	9.76	0	58.22	45.7	9.76	7.7
		$2*A1+2*A6$					[216]
C_4H_8		isobutene					
	132.4	5.92	0	44.72	41.8	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)
		$A7+2*A1+A5$						[216]
$C_4H_8Br_2O_2$			(*dl*) 2,3-dibromo-1,4-butanediol					
	363.2		29.29	0	80.64	75.9	29.29	27.6
		$2*A21+2*A2+2*A3*B3+2*A30*D30$						[226]
$C_4H_8Br_2O_2$			(*d*) 2,3-dibromo-1, 4-butanediol					
	388.2		33.89	0	87.3	75.9	33.89	29.5
		$2*A21+2*A2+2*A3*B3+2*A30*D30$						[226]
$C_4H_8Cl_2O$			1,5-dichloro-3-oxapentane					
	226.5		8.39	0	37.02	65.6	8.39	14.9
		$4*A2+2*A22*C22+A32$						[216]
$C_4H_8Cl_3O_4P$			dimethyl (2,2,2-trichloro-1-hydroxyethyl)phosphonate					
	351.0		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
		$3*A22*E22+A4*B4+A3*B3+A30*E30+2*A1+A75$						[216]
$C_4H_8N_2O_2$			N-acetylglycine amide					
	408.2		25.6	0	62.71	54.1	25.6	22.1
		$A1+A2+A61+A60$						[216]
$C_4H_8N_4O_4$			1,3-dinitro-1,3-diazacyclohexane					
	343		15.8	46.06				
	354		2.97	8.39	54.45	69.9	18.77	24.7
		$A14+3*A15+2*A120+2*A51*C51$						[147]
$C_4H_8N_6O_5$			1,5-dinitro-3-nitroso-1,3,5-triazacycloheptane					
	404		25.7	63.61				
	440		2.9	6.59	70.2	75.1	28.6	33.1
		$A14+4*A15+3*A120+2*A51+A52$						[147]
$C_4H_8N_8O_8$			1,3,5,7-tetranitro-1,3,5,7-tetrazocine					
	553.2		69.87	0	126.3	102.7	69.87	56.8
		$A14+5*A15+4*A120+4*A51$						[216]
$C_4H_8N_{12}O_6$			1,7-diazido-2,4,6-trinitro-2,4,6-triazaheptane					
	406		40.17	0	98.93	99.0	40.17	40.2
		$4*A2+3*A51+2*A46+3*A47$						[225]
C_4H_8O			2-butanone					
	186.5		8.39	0	45.27	46.9	8.39	8.7
		$2*A1+A2+A35$						[341]
C_4H_8O			butanal					
	176.8		11.09	61.09	62.8	53.5	11.09	9.4
		$A1+2*A2+A34$						[216, 84]
C_4H_8O			tetrahydrofuran					
	164.8		8.54	0	51.88	42.0	8.54	6.9
		$A14+2*A15+A112$						[215]
$C_4H_8O_2$			butanoic acid					
	264.7		11.07	0	41.82	45.2	11.07	12.0
		$A1+A2+A36+A2$						[215]
$C_4H_8O_2$			ethyl acetate					
	189.3		10.48	0	55.35	50.0	10.48	9.5
		$2*A1+A38+A2$						[215]
$C_4H_8O_2$			1,4-dioxane					
	272.9		2.35	8.79				
	284.1		12.84	45.19	53.97	46.9	15.2	13.3
		$A14+3*A15+2*A112$						[216]
$C_4H_8O_2S$			tetramethylene sulfone					
	288.6		5.35	18.55				
	301.6		1.43	4.73	23.29	30.4	6.78	9.2
		$A14+2*A15+A134$						[202]
$C_4H_8O_4$			tetroxane					
	385		22.6	0	58.58	56.8	22.6	21.9
		$5*A15+A14+4*A112$						[216]
C_4H_8S			thiacyclopentane					
	177.0		7.35	0	41.55	43.7	7.35	7.7
		$A14+2*A15+A131$						[136]
$C_4H_8S_2$			1,3-dithiane					
	316.4		0.8	2.53				
	327.2		14.4	44.01	46.54	50.3	15.2	16.5
		$A14+3*A15+2*A131$						[216]
$C_4H_8S_2$			1,4-dithiane					
	384.6		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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		$A14+3*A15+2*A131$					[216]
C_4H_9Br		1-bromobutane					
	160.4	9.23	57.57	57.57	63.1	9.23	10.1
		$3*A2*B2+A21+A1$					[216]
C_4H_9Br		*tert*-butyl bromide					
	208.6	5.65	27.08				
	231.5	1.05	4.52				
	256.1	1.97	7.68	39.33	47.4	8.66	12.2
		$3*A1+A21+A4*B4$					[216]
C_4H_9Br		2-bromobutane					
	160.3	6.88	0	42.92	50.2	6.88	8.0
		$2*A1+A2+A3*B3+A21$					[215]
C_4H_9Cl		*tert*-butyl chloride					
	182.9	1.87	10.25				
	219.3	5.88	26.82				
	248.1	1.97	7.95	45.02	40.7	9.82	10.1
		$3*A1+A4*B4+A22$					[136]
C_4H_9N		pyrrolidine					
	207.1	0.54	2.61				
	215.3	8.58	39.84	42.44	43.0	9.12	9.3
		$A121+A14+2*A15$					[216]
$C_4H_9NO_2$		2-amino-2-methylpropanediol					
	352.9	5	14.17				
	353.7	18.46	52.19				
	384.1	2.78	7.24	73.6	64.4	26.24	24.7
		$2*A2+A4*B4+2*A30*C30+A45+A1$					[274]
$C_4H_9NO_3$		2-methyl-2-nitro-1-propanol					
	310	17.2	55.47				
	361	3.74	10.35	65.82	55.3	20.93	20.0
		$2*A1+A4*B4+A2+A30*B30+A50$					[216]
$C_4H_9NO_3$		2-methyl-2-nitro-1,3-propanediol					
	352	25.72	73.08				
	424	3.84	9.07	82.14	60.7	29.57	25.7
		$A1+A4*B4+2*A2+2*A30*C30+A50$					[216]
C_4H_{10}		butane					
	107.6	2.07	19.06				
	134.9	4.66	34.56	53.62	49.4	6.73	6.7
		$2*A1+2*A2$					[216]
C_4H_{10}		isobutane					
	113.7	4.54	0	40.11	36.4	4.54	4.1
		$3*A1+A3$					[216]
$C_4H_{10}Cl_2Si$		dichlorodiethylsilane					
	174.1	8.96	0	51.45	54.7	8.96	9.5
		$2*A22*C22+2*A1+2*A2+A109$					[216]
$C_4H_{10}Hg$		diethyl mercury					
	181.5	10.5	0	57.87	57.8	10.5	10.5
		$2*A1+A104+2*A2$					[216]
$C_4H_{10}N_2O$		N-propylurea					
	381	14.63	0	38.4	54.4	14.63	20.7
		$2*A2+A1+A67$					[215]
$C_4H_{10}N_2O$		N-isopropylurea					
	429	17.5	40.79				
	375.5	2.31	6.15				
	280.8	1.41	5.02	51.97	48.0	21.22	13.5
		$2*A1+A3*B3+A67$					[138]
$C_4H_{10}N_2O$		1,1,3-trimethylurea					
	344.4	14.3	0	41.52	52.9	14.3	18.2
		$3*A1+A64$					[215]
$C_4H_{10}N_4O_4$		N-N′dimethyl-N,N′dinitro-1,2-ethanediamine					
	410	60.32	0	147.13	139.7	60.32	57.3
		$2*A1+2*A2+2*A51+2*A47$					[225]
$C_4H_{10}O$		butyl alcohol					
	183.9	9.28	0	50.46	47.3	9.28	8.7
		$3*A2*B2+A1+A30$					[215]
$C_4H_{10}O$		2-butanol					
	184.7	5.97	0	32.33	34.4	5.97	6.4
		$2*A1+A2+A3*B3+A30$					[76]
$C_4H_{10}O$		*tert*-butyl alcohol					
	286.1	0.83	2.9				

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)
	294.5	0.49	1.66				
	299.0	6.7	22.42	26.98	31.6	8.02	9.5
		3*A1+A4*B4+A30					[216]
$C_4H_{10}O$		(+)2-butanol					
	177.4	6	0	33.82	34.4	6	6.1
		2*A1+A2+A3*B3+A30					[76]
$C_4H_{10}O$		2-methyl-1-propanol					
	171.2	6.32	0	36.93	27.7	6.32	4.7
		2*A1+A2+A3+A30					[73]
$C_4H_{10}O$		methyl isopropyl ether					
	127.3	5.85	0	45.73	47.8	5.85	6.1
		3*A1+A32+A3*B3					[216]
$C_4H_{10}O$		diethyl ether					
	156.9	7.19	0	45.81	54.1	7.19	8.5
		2*A1+2*A2+A32					[75]
$C_4H_{10}O$		methyl propyl ether					
	134.0	7.67	0	57.24	54.1	7.67	7.3
		A32+2*A1+2*A2					[216]
$C_4H_{10}O_2$		1,4-dihydroxybutane					
	293.6	18.7	0	63.7	73.6	18.7	21.6
		4*A2*B2+2*A30*B30					[216]
$C_4H_{10}O_4$		1,2,3,4-tetrahydroxybutane					
	396	42.36	0	106.97	86.6	42.36	34.3
		2*A2+2*A3*B3+4*A30*D30					[216]
$C_4H_{10}S$		diethyl sulfide					
	169.2	11.9	0	70.47	51.5	11.9	8.7
		2*A1+2*A2+A84					[216]
$C_4H_{10}S$		methyl propyl sulfide					
	160.2	9.91	0	61.88	51.5	9.91	8.7
		2*A1+2*A2+A84					[216]
$C_4H_{10}S$		isopropyl methyl sulfide					
	171.7	9.36	0	54.5	56.3	9.36	9.7
		3*A1+A3*B3+A84					[216]
$C_4H_{10}S$		isobutyl mercaptan					
	128.3	4.98	0	38.83	48.9	4.98	6.3
		2*A1+A3+A2+A86					[216]
$C_4H_{10}S$		*n*-butyl mercaptan					
	157.5	10.46	0	66.44	68.6	10.46	10.8
		A1+3*A2*B2+A86					[216]
$C_4H_{10}S$		*tert*-butyl mercaptan					
	151.6	4.07	26.83				
	157	0.65	4.13				
	199.4	0.97	4.87				
	274.4	2.48	9.04	44.87	52.9	8.17	14.5
		3*A1+A4*B4+A86					[216]
$C_4H_{10}S$		2-butanethiol					
	133.0	6.48	0	48.7	55.5	6.48	7.4
		2*A1+A2+A3*B3+A86					[216]
$C_4H_{10}S_2$		diethyl disulfide					
	171.6	9.4	0	54.77	59.0	9.4	10.1
		2*A1+2*A2+A85					[216]
$C_4H_{10}Zn$		diethyl zinc					
	148.4	0.28	1.86				
	237.0	16.63	70.19	72.05	60.5	17.52	14.3
		2*A1+2*A2+A111					[216, 96]
$C_4H_{11}N$		*tert*-butyl amine					
	91.3	0.11	1.24				
	202.3	6.05	29.92				
	206.2	0.88	4.28	35.44	51.3	7.05	4.7
		3*A1+A4*B4+A45					[126]
$C_4H_{11}NO_2$		2-amino-2-methylpropane-1,3-diol					
	352	25.21	71.61				
	384	2.99	7.79	79.39	64.4	5.4	24.7
		2*A2+A4*B4+A1+2*A30*C30+A45					[216]
$C_4H_{11}NO_3$		2-amino-2-hydroxymethylpropane-1,3-diol					
	443.6	2.41	5.43				
	407.5	33.42	82.01	87.45	88.7	40.87	36.1
		3*A2+A4*B4+3*A30*D30+A45					[34]
$C_4H_{12}Ge$		tetramethylgermanium					
	184.4	7.45	0	40.4	35.1	7.45	6.5
		4*A1+A102					[54]

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)
$C_4H_{12}N_2$		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
		2*A45+2*A1+A2+A4*B4					[50]
$C_4H_{12}Pb$		tetramethyllead					
	242.9	10.8	0	44.45	40.2	10.8	9.8
		4*A1+A106					[216]
$C_4H_{12}Si$		teramethylsilane					
	174.0	6.74	0	38.73	43.2	6.74	7.5
		4*A1+A109					[216]
$C_4H_{12}Sn$		tetramethyltin					
	218.2	9.23	0	42.32	46.1	9.23	10.1
		4*A1+A110					[166, 125]
$C_5F_{11}N$		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
		A14+3*A15+5*A17+A119+11*A28					[216]
$C_5F_{13}N$		perfluoromethyldiethylamine					
	149.7	7.16	0	47.83	49.3	7.16	7.2
		4*A26+5*A4*B4+A43+9*A25					[216]
$C_5H_2Cl_3O$		3,5,6-trichloro-2-pyridinol					
	448.1	25.97	0	57.55	57.2	25.79	25.6
		3*A22*E22+A31+A41+A10+4*A12					[215]
$C_5H_3F_7O_2$		methyl perfluorobutanoate					
	191.4	11.7	0	61.49	62.3	11.77	11.8
		A1+A38+4*A26+3*A25+3*A4*B4					[216]
$C_5H_4O_2$		furfural					
	235.1	14.37	0	61.11	45.0	14.37	10.6
		A14+2*A15+2*A18+A18*B18+A19+A34+A112					[216]
$C_5H_5F_3O_2$		trifluoromethyl (2-hydroxy-1-propenyl)ketone					
	232.4	8.45	0	36.36	53.4	8.45	12.4
		A4*B4+3*A25+A1+A6*B6+A7+A30*E30+A35					[216]
C_5H_5N		pyridine					
	231.5	8.28	0	35.75	48.0	8.28	11.1
		5*A10+A41					[216]
C_5H_6		cyclopentadiene					
	176.6	8.01	0	45.36	34.3	8.01	6.1
		A14+2*A15+4*A18					[216]
$C_5H_6N_2$		1,3-dicyanopropane					
	244.2	12.59	0	51.55	63.5	12.59	15.5
		2*A56+3*A2*B2					[216]
$C_5H_6N_2$		2,2-dicyanopropane					
	302.6	9.87	32.59				
	307.5	4.05	13.18	45.17	47.8	13.92	14.7
		2*A56+A4*B4+2*A1					[216]
$C_5H_6N_2$		4-aminopyridine					
	429.9	20.07	0	46.68	54.5	20.07	23.4
		4*A10+A12+A41+A45					[221]
$C_5H_6N_2O_2$		thymine					
	321.3	17.51	0	54.5	52.1	17.51	16.7
		A14+3*A15+2*A124+A18*B18+A19+A1					[216]
C_5H_6O		2-methylfuran					
	181.9	8.55	0	47.03	41.0	8.55	7.5
		A1+A14+2*A15+2*A18+A19+A112+A18*B18					[106]
$C_5H_6O_2$		furfuryl alcohol					
	258.6	13.1	0	50.75	48.7	13.1	12.6
		A2+A14+2*A15+2*A18+A19+A112+A18*B18+A30*B30					[216]
C_5H_6S		2-methylthiophene					
	207.8	9.47	0	45.57	42.7	9.47	8.9
		A14+2*A15+A131+2*A18+A19+A1+A18*B18					[275]
C_5H_6S		3-methylthiophene					
	204.2	10.54	0	51.62	41.2	10.54	8.4
		A14+2*A15+A131+A1+A19+2*A18*B18+A18					[136]
C_5H_7N		N-methylpyrrole					
	216.9	7.82	0	36.07	29.6	7.82	6.4
		A14+2*A15+A1+2*A18+2*A18*B18+A119					[216]
$C_5H_7NO_2$		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)
		2*A2+A1+A38+A56						[216]
C_5H_8			spiropentane					
	166.1		6.43	0	38.7	28.5	6.43	4.7
		2*A14+A17−A15						[216]
C_5H_8			1-*cis*-3-pentadiene					
	132.4		5.64	0	42.61	50.7	5.64	6.7
		A1+A5+3*A6						[216]
C_5H_8			*trans*-1,3-pentadiene					
	185.7		7.14	0	38.46	50.7	7.14	9.4
		A1+A5+3*A6						[216]
C_5H_8			1,4-pentadiene					
	124.3		6.14	0	49.41	52.3	6.14	6.5
		A2+2*A5+2*A6						[216]
C_5H_8			2-methyl-1,3-butadiene					
	127.3		4.92	0	38.68	34.7	4.92	4.4
		A1+A7+A5+2*A6						[216]
C_5H_8			3-methyl-1,2-butadiene					
	159.5		7.95	0	49.84	39.0	7.95	6.2
		2*A1+A9+A5+A7						[216]
C_5H_8			2,3-pentadiene					
	147.5		6.13	0	44.82	42.9	6.13	6.3
		2*A1+2*A6+A9						[216]
C_5H_8			1,2-pentadiene					
	135.9		7.56	0	55.73	44.5	7.56	6.1
		A1+A2+A5+A6+A9						[216]
C_5H_8			cyclopentene					
	87.07		0.48	5.51				
	138.1		3.36	24.32	29.83	37.6	3.84	5.2
		A14+2*A15+2*A18						[216]
C_5H_8			methylenecyclobutane					
	138.5		5.86	0	42.31	42.2	5.86	5.8
		A14+A15+A5+A19						[216]
$C_5H_8Br_4$			pentaerythrityl tetrabromide					
	433.5		27.97	0	64.52	63.9	27.97	27.7
		4*A2+A4+4*A21						[216]
$C_5H_8Cl_2O$			3,3-bis-(chloromethyl)oxacyclobutane					
	292.2		16.95	0	58	50.4	16.95	14.7
		2*A2+2*A22*C22+A15+A14+A17+A112						[216]
$C_5H_8F_4$			pentaerythritol tetrafluoride					
	367.4		5.14	13.97				
	249.4		13.21	53.14	67.11	44.3	18.35	11.1
		4*A2+4*A27+A4						[216]
$C_5H_8O_2$			δ-valerolactone					
	118		0.46	3.88				
	135		0.3	2.2				
	200		0.2	0.9				
	263		10.53	40.04	43.1	47.6	11.29	12.5
		3*A15+A14+A115						[32]
$C_5H_8O_2$			methyl methacrylate					
	225		12.24	0	54.4	49.5	12.24	11.1
		2*A1+A38+A7+A5						[216]
$C_5H_8O_2$			acetylacetone enol					
	254.8		14.5	0	56.91	66.0	14.5	16.8
		2*A1+A35*B35+A30*B30+A6*B6+A7						[60]
$C_5H_8O_3$			levulinic acid					
	306.2		9.22	0	30.11	52.5	9.22	16.1
		A1+2*A2+A35*B35+A36*B36						[215]
$C_5H_8O_4$			glutaric acid					
	348.5		2.46	7.07				
	371		20.9	56.33	63.4	60.2	23.36	22.3
		3*A2*B2+2*A36*B36						[216]
C_5H_9Cl			chlorocyclopentane					
	169.4		7.63	45.05				
	180		0.64	3.54	48.59	36.8	8.27	6.6
		A14+2*A15+A16+A22						[35]
C_5H_9N			2-cyano-2-methylpropane					
	213		0.23	1.09				
	232.7		1.91	7.78				
	292.1		9.29	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)
		3*A1+A4*B4+A56					[216]
$C_5H_{10}ClNO$		2-chloro-N-isopropylacetamide					
	351.3	26.05	0	74.15	50.1	26.05	17.6
		2*A1+A2+A3*B3+A60+A22*B22					[221]
C_5H_9NO		2-piperidone					
	342.3	16.1	0	47.02	47.2	16.1	16.2
		A14+3*A15+A124					[227]
C_5H_{10}		cyclopentane					
	122	4.9	40.13				
	138	0.34	2.49				
	179.7	0.6	3.35	45.96	40.8	5.84	7.3
		A14+2*A15					[216]
C_5H_{10}		*cis*-2-pentene					
	121.8	7.11	0	58.39	52.8	7.11	6.4
		2*A1+A2+2*A6					[215]
C_5H_{10}		*trans*-2-pentene					
	133.0	8.35	0	62.82	52.8	8.35	7.0
		2*A1+A2+2*A6					[215]
C_5H_{10}		1-pentene					
	107.9	5.81	55	53.82	54.4	5.81	5.9
		A1+2*A2+A5+A6					[215]
C_5H_{10}		3-methyl-1-butene					
	104.7	5.36	0	51.19	41.4	5.36	4.3
		2*A1+A3+A5+A6					[216]
C_5H_{10}		2-methyl-2-butene					
	139.4	7.60	0	54.47	59.4	7.60	8.3
		3*A1+A7+A5					[216]
C_5H_{10}		2-methyl-1-butene					
	135.6	7.91	0	58.34	48.9	7.91	6.6
		2*A1+A2+A7+A5					[216]
C_5H_{10}		methylcyclobutane					
	138.6	5.76	0	41.56	39.9	5.76	5.5
		A1+A14+A15+A16					[215]
$C_5H_{10}N_2O_2$		N-acetyl-L-alanine amide					
	431	21.7	0	50.35	54.9	21.7	23.7
		2*A1+A3*B3+A61+A60					[216]
$C_5H_{10}N_2O_2S$		5-methyl N-(methylcarbamoyloxy)thioacetimidate					
	352.7	21.73	0	61.61	53.0	21.73	18.7
		3*A1+A69+A42+A7+A84					[221]
$C_5H_{10}N_2O_3$		alanylglycine (with decomp)					
	508.0	56.6	0	111.43	67.7	56.6	34.4
		A1+A2+A3*B3+A45+A36*C36+A60					[216]
$C_5H_{10}N_4O_4$		1,3-dinitro-1,3-diazacycloheptane					
	369	21.8	59.08				
	374	2.8	7.49	66.57	73.6	24.6	27.5
		A14+4*A15+2*A120+2*A51					[147]
$C_5H_{10}O$		pivaldehyde					
	158.5	0.5	3.15				
	183.9	4.81	26.15				
	272.1	2.52	9.26	38.56	51.4	7.83	14.0
		3*A1+A4*B4+A34					[163]
$C_5H_{10}O$		3-pentanone					
	118.5	0.11	0.96				
	180	0.01	0.04				
	234.2	11.59	49.5	50.5	54.0	11.71	12.7
		2*A1+2*A2+A35					[341]
$C_5H_{10}O$		2-pentanone					
	110	2.09	2.18				
	196.3	10.63	54.14	56.32	54.0	12.72	10.6
		2*A1+2*A2+A35					[341]
$C_5H_{10}O$		cyclopentanol					
	202.8	3.71	18.28				
	257.4	1.54	5.98	24.27	27.8	5.24	7.2
		A14+2*A15+A16+A30					[216]
$C_5H_{10}O$		isopropyl methyl ketone					
	180.0	9.34	0	51.9	47.5	9.34	8.5
		3*A1+A3*B3+A35					[216]
$C_5H_{10}O_2$		pentanoic acid					
	239.5	14.16	0	59.14	58.9	14.16	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_5H_{10}O_2$		2,2-dimethylpropanoic acid (pivalic acid)					
	278.3	8.18	29.39				
	309.1	2.27	7.34	36.74	43.3	10.45	13.4
		3*A1+A4*B4+A36					[180]
$C_5H_{10}O_4$		2,2-bis-hydroxymethylpropanoic acid					
	426	38.5	90.37				
	468	3.59	7.68	98.05	73.0	42.09	34.2
		A1+2*A2+A4*B4+A36*C36+2*A30*C30					[216]
$C_5H_{10}O_5$		pentacycloformaldehyde					
	334	21.9	0	65.6	65.4	21.9	21.8
		7*A15+A14+5*A112					[216]
$C_5H_{10}S$		2-methylcyclothiapentane					
	172.4	8.87	0	51.48	46.5	8.87	8.0
		A14+2*A15+A1+A16+A131					[216]
$C_5H_{10}S$		3-methylcyclothiapentane					
	192	10.37	0	54	46.5	10.37	8.9
		A14+2*A15+A1+A16+A131					[216]
$C_5H_{10}S$		thiacyclohexane					
	201.4	1.1	5.44				
	240.0	7.77	32.38				
	292.3	2.45	8.37	46.19	47.4	11.32	13.9
		A14+3*A15+A131					[216]
$C_5H_{10}S$		cyclopentanethiol					
	155.4	7.83	0	50.38	49.1	7.83	7.6
		A14+2*A15+A86+A16					[288]
$C_5H_{11}Br$		1-bromopentane					
	185.1	14.37	77.61	77.61	72.5	14.37	13.4
		4*A2*B2+A1+A21					[216]
$C_5H_{11}N$		cyclopentylamine					
	184.5	0.48	2.58				
	190.4	8.31	43.65	46.23	47.4	8.79	9.0
		A14+2*A15+A45+A16					[216]
$C_5H_{11}NO$		piperidine					
	262.1	14.85	0	56.64	46.7	14.85	12.2
		A14+3*A15+A121					[216]
$C_5H_{11}NO_2$		N-methylmorpholine-N-oxide					
	457.4	18.8	0	41.1	41.1	18.8	18.8
		A14+3*A15+A112+A122+A1					[151]
$C_5H_{11}NO_2$		2-amino-2-methyl-1,3-propanediol					
	351.3	24.68	70.26				
	383.6	2.73	7.12	77.38	64.4	27.41	24.7
		A1+2*A2+A4*B4+2*A30*C30+A45					[216]
$C_5H_{11}NO_3S$		2-methyl-2-(methylsulfonyl)propanal oxime					
	382.0	27.12	0	71.01	47.6	27.12	18.2
		3*A1+A4*B4+A6*B6+A88+A53					[221]
C_5H_{12}		pentane					
	143.5	8.4	0	58.58	63.2	8.4	9.1
		2*A1+3*A2*B2					[215]
C_5H_{12}		2-methylbutane					
	113.4	5.13	0	45.23	43.5	5.13	4.9
		3*A1+A3+A2					[216]
C_5H_{12}		2,2-dimethylpropane					
	140	2.58	18.41				
	256.5	3.26	12.69	31.1	35.5	5.83	5.0
		4*A1+A4					[216]
$C_5H_{12}NO_3PS$		O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] phosphorodithioate					
	321.0	20.49	0	63.85	51.7	20.49	16.6
		3*A1+A60+A2+A80					[221]
$C_5H_{12}N_2O$		N-butylurea					
	313.1	7.02	22.42				
	344.9	0.88	2.55				
	369.3	14.55	39.4	64.37	68.1	22.45	25.1
		3*A2*B2+A1+A67					[215]
$C_5H_{12}N_2O$		N-*tert*-butylurea					
	249	0.1	0.41				
	449.8	33.13	73.65	74.06	52.4	33.23	23.6
		3*A1+A4*B4+A67					[215]
$C_5H_{12}N_2O$		1,1-diethylurea					
	197.3	2.07	10.49				
	342.3	16.78	49.02	59.51	68.9	18.85	23.6
		2*A1+2*A2+A65					[215, 124, 138]

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)
$C_5H_{12}N_2O$		1,3-diethylurea					
	339.4	1.87	5.51				
	383.4	12.46	32.5	38.01	50.9	14.33	19.5
		2*A1+A66+2*A2					[215, 124, 138]
$C_5H_{12}N_2O$		tetramethylurea					
	272.2	13.4	0	49.23	51.0	13.4	13.9
		4*A1+A63					[216]
$C_5H_{12}N_2O_2$		N-methyl-N-nitrobutanamine					
	331	37.56	0	113.46	101.7	37.56	33.7
		2*A1+3*A2+A51+A47					[225]
$C_5H_{12}O$		2,2-dimethyl-1-propanol					
	146	1.96	13.43				
	213	0.17	0.79				
	264	4.46	16.88	31.1	26.8	6.59	7.1
		3*A1+A4+A2+A30					[277]
$C_5H_{12}O$		1-pentanol					
	195.6	10.5	0	53.7	56.7	10.5	11.1
		A1+4*A2*B2+A30					[216]
$C_5H_{12}O$		methyl *tert*-butyl ether					
	164.6	7.6	0	46.19	52.2	7.6	8.6
		4*A1+A4*B4+A32					[216]
$C_5H_{12}O$		ethyl propyl ether					
	145.7	8.39	0	57.61	61.3	8.39	8.9
		2*A1+3*A2+A32					[216]
$C_5H_{12}O$		methyl *n*-butyl ether					
	157.5	10.85	0	68.9	61.3	10.85	9.7
		2*A1+3*A2+A32					[216]
$C_5H_{12}O_2$		1,5-pentanediol					
	248	15.72	0	63.6	82.9	15.72	20.6
		5*A2*B2+2*A30*B30					[216]
$C_5H_{12}O_2$		2-methyl-2-butanol					
	146	1.96	13.44				
	213	0.17	0.78				
	264	4.46	16.88	31.1	38.8	6.59	10.2
		3*A1+A4*B4+A2+A30					[216]
$C_5H_{12}O_2$		2,2-dimethyl-1,3-propanediol					
	315.2	13.8	43.78				
	403.2	4.6	11.41	55.19	50.8	18.4	20.5
		2*A1+2*A2+A4+2*A30*B30					[90]
$C_5H_{12}O_3$		2-hydroxymethyl-2-methyl-1,3-propanediol					
	354	23.17	65.46				
	470	5.38	11.44	76.91	55.1	28.55	25.9
		A1+3*A2+A4+3*A30*C30					[216]
$C_5H_{12}O_4$		pentaerythritol					
	460.4	43.93	95.4				
	538.7	7.11	13.2	108.78	85.4	51.04	46.0
		A4+4*A2+4*A30*D30					[216]
$C_5H_{12}O_5$		1,2,3,4,5-pentahydroxypentane (Ribitol)					
	374.7	37.6	0	100.35	90.4	37.6	39.9
		2*A2+3*A3*B3+5*A30*E30					[216]
$C_5H_{12}O_5$		1,2,3,4,5-pentahydroxypentane (Xylitol)					
	365.7	37.4	0	102.27	90.4	37.4	33.1
		2*A2+3*A3*B3+5*A30*E30					[216]
$C_5H_{12}O_5$		1,2,3,4,5-pentahydroxypentane (D-Arabitol)					
	379.4	38.9	0	102.53	90.4	38.9	34.3
		2*A2+3*A3*B3+5*A30*E30					[216]
$C_5H_{12}S$		methyl *tert*-butyl sulfide					
	190.8	8.41	0	44.1	49.6	8.41	9.5
		4*A1+A4*B4+A84					[216]
$C_5H_{12}S$		ethyl propyl sulfide					
	156.1	10.58	0	67.8	58.7	10.58	9.2
		2*A1+3*A2+A84					[216]
$C_5H_{12}S$		methyl butyl sulfide					
	175.6	12.45	0	70.9	58.7	12.45	10.3
		2*A1+3*A2+A84					[136]
$C_5H_{12}S$		3-methyl-1-butanethiol					
	139.6	7.41	0	53.05	56.1	7.41	7.8
		2*A1+A3+2*A2+A86					[216]
$C_5H_{12}S$		1-pentanethiol					
	197.5	17.53	0	88.78	77.9	17.53	15.4

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]
$C_5H_{12}SO_2$		*tert*-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}		*n*-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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
C_6HCl_5O		pentachlorophenol					
	462.5	17.15	0	37.08	56.3	17.15	26.0
		5*A22*F22+A31+6*A12					[215, 191]
C_6HF_5		pentafluorobenzene					
	225.7	10.88	0	48.24	53.2	10.88	12.0
		5*A24+5*A12+A10					[215]
C_6HF_5O		pentafluorophenol					
	287	1.16	4.04				
	310.6	16.41	52.83	56.87	58.5	17.57	18.2
		6*A12+A31+5*A24					[72]
$C_6H_2Br_4$		1,2,4,5-tetrabromobenzene					
	306.8	0.34	1.09				
	453.1	27.88	61.53	62.62	55.1	28.22	25.0
		4*A21+4*A12+2*A10					[216]
$C_6H_2Cl_4$		1,2,3,4-tetrachlorobenzene					
	320	17	0	53.13	49.6	17	15.9
		4*A12+2*A10+4*A22*D22					[215]
$C_6H_2Cl_4$		1,2,4,5-tetrachlorobenzene					
	421.2	24.1	0	57.22	49.6	24.1	20.9
		4*A12+2*A10+4*A22*D22					[215]
$C_6H_2Cl_4$		1,2,3,5-tetrachlorobenzene					
	323.9	19	0	58.66	49.6	19	16.1
		4*A12+2*A10+4*A22*D22					[215]
$C_6H_2Cl_5N$		pentachloroaniline					
	505.8	18.7	0	36.97	57.4	18.7	29.0
		6*A12+5*A22*F22+A45					[215]
$C_6H_2F_4$		1,2,3,4-tetrafluorobenzene					
	233.3	10.93	0	46.85	51.4	10.93	12.0
		4*A12+2*A10+4*A24					[65]
$C_6H_2F_4$		1,2,3,5-tetrafluorobenzene					
	226.9	10.67	0	47.01	51.4	10.67	11.7
		4*A12+2*A10+4*A24					[65]
$C_6H_2F_4$		1,2,4,5-tetrafluorobenzene					
	277	15.05	0	54.31	51.4	15.05	14.3
		4*A12+2*A10+4*A24					[65]
$C_6H_2F_5N$		pentafluoroaniline					
	287.4	3.94	13.71				
	306.8	14.27	46.51	60.22	59.6	18.21	18.3
		5*A24+A45+6*A12					[216]
$C_6H_3BrCl_2O$		4-bromo-2,5-dichlorophenol					
	343.4	22.11	0	64.39	55.0	22.11	18.9
		2*A10+4*A12+2*A22*D22+A21+A31					[221]
$C_6H_3Br_3O$		2,4,6-tribromophenol					
	366.2	18.52	0	50.57	57.8	18.52	21.2
		4*A12+2*A10+3*A21+A31					[215]
$C_6H_3Cl_3$		1,2,3-trichlorobenzene					
	326.9	20.5	0	62.71	48.4	20.5	15.8
		3*A10+3*A12+3*A22*C22					[215]
$C_6H_3Cl_3$		1,3,5-trichlorobenzene					
	336.7	18.2	0	54.05	48.4	18.2	16.3
		3*A10+3*A12+3*A22*C22					[215]
$C_6H_3Cl_3O$		2,4,5-trichlorophenol					
	340.3	21.59	0	63.44	53.7	21.59	18.3
		4*A12+2*A10+3*A22*D22+A31					[221]
$C_6H_3Cl_4N$		2-chloro-6-(trichloromethyl)pyridine					
	337.2	20.3	0	60.2	58.0	20.3	19.6
		3*A10+A41+A11+A12+A4*B4+4*A22*E22					[216]
$C_6H_3N_3O_6$		1,3,5-trinitrobenzene					
	370	1.9	5.13				
	380.3	14.8	38.95	44.08	53.0	16.71	20.2
		3*A10+3*A12+3*A50*C50					[216]
$C_6H_3N_3O_7$		picric acid					
	394.1	17.1	0	43.39	58.4	17.1	23.0
		2*A10+4*A12+3*A50+A31					[216]
$C_6H_3N_3O_8$		2,4,6-trinitroresorcinol					
	454.8	33.5	0	73.66	63.7	33.5	29.0
		A10+5*A12+2*A31+3*A50					[216]
C_6H_4BrCl		1,2-bromochlorobenzene					

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)
	260.6	12.37	0	47.47	48.4	12.37	12.6
		A22*B22+A21+2*A12+4*A10					[216]
C_6H_4BrCl		1,3-bromochlorobenzene					
	252.0	12.29	0	48.77	48.4	12.29	12.2
		A22*B22+A21+2*A12+4*A10					[216]
C_6H_4BrCl		1,4-bromochlorobenzene					
	337.8	18.76	0	55.54	48.4	18.76	16.4
		A22*B22+A21+2*A12+4*A10					[216]
C_6H_4BrI		1,2-bromoiodobenzene					
	294.2	14.42	0	49.01	51.6	14.42	15.2
		4*A10+2*A12+A21+A29					[215]
C_6H_4BrI		1,3-bromoiodobenzene					
	282.5	12.16	0	43.04	51.6	12.16	14.6
		4*A10+2*A12+A21+A29					[215]
C_6H_4BrI		1,4-bromoiodobenzene					
	363.3	19.13	0	52.66	51.6	19.13	18.8
		4*A10+2*A12+A21+A29					[215]
$C_6H_4Br_2$		1,2-dibromobenzene					
	275	12.61	0	45.58	49.8	12.61	13.7
		4*A10+2*A12+2*A21					[215]
$C_6H_4Br_2$		1,3-dibromobenzene					
	266.3	13.21	0	49.61	49.8	13.21	13.3
		4*A10+2*A12+2*A21					[215]
$C_6H_4Br_2$		1,4-dibromobenzene					
	360.1	20.04	0	55.65	49.8	20.04	17.9
		2*A21+4*A10+2*A12					[215]
$C_6H_4Br_2O$		2,4-dibromophenol					
	313	14.64	0	46.79	55.2	14.64	17.3
		3*A10+3*A12+2*A21+A31					[215]
$C_6H_4ClNO_2$		1,2-chloronitrobenzene					
	308.2	19.08	0	61.9	48.6	19.08	15.0
		4*A10+2*A12+A22*B22+A50					[228]
$C_6H_4ClNO_2$		1,4-nitrochlorobenzene					
	354.6	11.85	0	33.42	48.6	11.85	17.2
		4*A10+2*A12+A50+A22*B22					[216]
$C_6H_4ClNO_2$		1,3-nitrochlorobenzene					
	317.6	19.37	0	60.99	48.6	19.37	15.4
		A22*B22+A50+4*A10+2*A12					[215]
$C_6H_4Cl_2$		1,2-dichlorobenzene					
	256.5	12.93	0	50.41	47.1	12.93	12.1
		4*A10+2*A12+2*A22*B22					[215]
$C_6H_4Cl_2$		1,3-dichlorobenzene					
	248.4	12.64	0	50.89	47.1	12.64	11.7
		4*A10+2*A12+2*A22*B22					[215]
$C_6H_4Cl_2$		1,4-dichlorobenzene					
	326	18.16	0	55.65	47.1	18.16	15.3
		2*A22*B22+4*A10+2*A12					[215]
$C_6H_4Cl_2N_2O_2$		2,6-dichloro-4-nitroaniline					
	466.8	32.64	0	69.92	56.4	32.64	26.3
		4*A12+2*A10+A45+2*A22*D22+A50					[215]
$C_6H_4Cl_2O$		2,3-dichlorophenol					
	330	21.36	0	64.73	52.4	21.36	17.3
		3*A10+3*A12+A31+2*A22*C22					[215]
$C_6H_4Cl_2O$		2,4-dichlorophenol					
	318	20.09	0	63.18	52.4	20.09	16.7
		3*A10+3*A12+A31+2*A22*C22					[216]
$C_6H_4Cl_2O$		2,5-dichlorophenol					
	331	22.43	0	67.76	52.4	22.43	17.4
		3*A10+3*A12+A31+2*A22*C22					[216]
$C_6H_4Cl_2O$		2,6-dichlorophenol					
	340	22.14	0	65.12	52.4	22.14	17.8
		3*A10+3*A12+A31+2*A22*C22					[216]
$C_6H_4Cl_2O$		3,4-dichlorophenol					
	341	20.93	0	61.38	52.4	20.93	17.9
		3*A10+3*A12+A31+2*A22*C22					[216]
$C_6H_4Cl_2O$		3,5-dichlorophenol					
	341	20.51	0	60.15	52.4	20.51	17.9
		3*A10+3*A12+A31+2*A22*C22					[216]
$C_6H_4F_2$		1,2-difluorobenzene					

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)
	226	11.05	0	48.95	48.0	11.05	10.8
		4*A10+2*A12+2*A24					[216]
$C_6H_4F_2$		1,3-difluorobenzene					
	186.8	0.83	4.43				
	204.0	8.58	42.05	46.48	48.0	9.4	9.8
		2*A24+2*A12+4*A10					[216]
$C_6H_4I_2$		1,2-diiodobenzene					
	296.6	14.01	0	47.24	53.5	14.01	15.9
		2*A29+2*A12+4*A10					[215]
$C_6H_4I_2$		1,3-diiodobenzene					
	307.4	15.93	0	51.82	53.5	15.93	16.4
		2*A29+2*A12+4*A10					[215]
$C_6H_4I_2$		1,4-diiodobenzene					
	402	22.37	0	55.65	53.5	22.37	21.5
		2*A29+2*A12+4*A10					[215]
$C_6H_4N_2O_4$		1,2-dinitrobenzene					
	396.1	22.84	0	57.66	50.2	22.84	19.9
		4*A10+2*A12+2*A50					[216]
$C_6H_4N_2O_4$		1,3-dinitrobenzene					
	363.2	17.36	0	47.82	50.2	17.36	18.2
		4*A10+2*A12+2*A50					[215]
$C_6H_4N_2O_4$		1,4-dinitrobenzene					
	446.7	28.12	0	62.93	50.2	28.12	22.4
		4*A10+2*A12+2*A50					[215]
$C_6H_4N_2O_5$		2,3-dinitrophenol					
	417	26.24	0	62.93	55.5	26.24	23.2
		3*A10+3*A12+2*A50+A31					[216]
$C_6H_4N_2O_5$		2,4-dinitrophenol					
	388	24.17	0	62.29	55.5	24.17	21.6
		3*A10+3*A12+2*A50+A31					[216]
$C_6H_4N_2O_5$		2,5-dinitrophenol					
	381	23.73	0	62.28	55.5	23.73	21.2
		3*A10+3*A12+2*A50+A31					[216]
$C_6H_4N_2O_5$		2,6-dinitrophenol					
	336	19.58	0	58.27	55.5	19.58	18.7
		3*A10+3*A12+2*A50+A31					[216]
$C_6H_4N_2O_5$		3,4-dinitrophenol					
	407	25.37	0	62.33	55.5	25.37	22.6
		3*A10+3*A12+2*A50+A31					[216]
$C_6H_4O_2$		*p*-benzoquinone					
	388	18.45	0	47.56	29.4	18.45	11.4
		3*A15+A14+4*A18*B18+2*A114					[215]
C_6H_5Br		bromobenzene					
	242.4	10.7	0	44.2	47.1	10.7	11.4
		5*A10+A12+A21					[216]
C_6H_5BrO		4-bromophenol					
	336	16.57	0	49.32	52.5	16.57	17.6
		A21+4*A10+2*A12+A31					[216]
C_6H_5Cl		chlorobenzene					
	227.9	9.55	0	41.92	40.4	9.55	9.2
		5*A10+A22+A12					[216]
C_6H_5ClO		2-chlorophenol					
	276	0.09	0.33				
	283	12.52	44.24	44.57	51.2	12.61	14.5
		4*A10+2*A12+A22*B22+A31					[215]
C_6H_5ClO		3-chlorophenol					
	305.8	14.91	0	48.76	51.2	14.91	15.6
		4*A10+2*A12+A22*B22+A31					[215]
C_6H_5ClO		4-chlorophenol					
	315.9	14.07	0	44.54	51.2	14.07	16.2
		4*A10+2*A12+A22*B22+A31					[215]
$C_6H_5Cl_2N$		2,6-dichloro-4-benzenamine					
	467.2	29.48	0	63.11	53.5	29.48	25.0
		3*A10+3*A12+2*A22*C22+A45					[221]
$C_6H_5Cl_3Si$		phenyltrichlorosilane					
	233.4	11.66	0	49.96	48.9	11.66	11.4
		5*A10+A11+3*A22*D22+A109					[216]
C_6H_5F		fluorobenzene					

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)
	230.9	11.31	0	48.95	46.2	11.31	10.7
		5*A10+A12+A24					[250]
C_6H_5I		iodobenzene					
	241.8	9.75	0	40.31	49.0	9.75	11.8
		5*A10+A12+A29					[216]
$C_6H_5NO_2$		picolinic acid					
	411	30	0	72.99	49.2	30	20.2
		4*A10+A12+A41+A36*B36					[216]
$C_6H_5NO_2$		nicotinic acid					
	452	0.78	1.73				
	510	26.7	52.35	54.08	49.2	27.48	25.1
		4*A10+A12+A41+A36*B36					[182]
$C_6H_5NO_2$		isonicotinic acid					
	593	135	0	227.66	49.2	135	29.2
		4*A10+A12+A41+A36*B36					[216]
$C_6H_5NO_2$		nitrobenzene					
	278.8	12.12	0	43.5	47.3	12.12	13.2
		5*A10+A12+A50					[216]
$C_6H_5NO_3$		*o*-nitrophenol					
	318.2	17.45	0	54.83	52.7	17.45	16.8
		4*A10+2*A12+A50+A31					[215,188]
$C_6H_5NO_3$		*m*-nitrophenol					
	371.2	19.19	0	51.7	52.7	19.19	19.6
		4*A10+2*A12+A50+A31					[215,188]
$C_6H_5NO_3$		*p*-nitrophenol					
	388.2	18.25	0	47.02	52.7	18.25	20.5
		4*A10+2*A12+A50+A31					[216,188]
C_6H_6		benzene					
	278.7	9.87	0	35.4	44.5	9.87	12.4
		6*A10					[216]
$C_6H_6Cl_6$		1α,2α,3β,4α,5α,6β-hexachlorocyclohexane					
	386.8	22.13	0	57.23	53.2	22.13	20.6
		A14+3*A15+6*A16+6*A22*F22					[221]
$C_6H_6Cl_6$		1α,2α,3β,4α,5α,6β-hexachlorocyclohexane (lindane)					
	388.9	15.9	0	40.88	53.2	15.9	20.7
		A14+3*A15+6*A16+6*A22*F22					[221]
$C_6H_6N_2O_2$		2-nitroaniline					
	342.5	16.11	0	47.0	53.8	16.11	18.5
		4*A10+A45+A50+2*A12					[216]
$C_6H_6N_2O_2$		3-nitroaniline					
	387	23.68	0	61.16	53.8	23.68	20.8
		4*A10+A45+A50+2*A12					[216]
$C_6H_6N_2O_2$		4-nitroaniline					
	420.7	21.09	0	50.1	53.8	21.09	22.6
		4*A10+A45+A50+2*A12					[216]
$C_6H_6N_6O_{14}$		2,2,2-trinitroethyl 4,4,4-trinitrobutyrate					
	362.7	25.94	71.52				
	366.5	6.69	18.27	89.79	89.7	32.64	32.9
		3*A2+2*A4*B4+A38+6*A50					[122]
C_6H_6O		phenol					
	314	11.51	0	36.82	49.9	11.51	15.7
		5*A10+A31+A12					[216]
$C_6H_6O_2$		1,4-dihydroxybenzene					
	445	26.48	0	59.5	59.5	26.48	25.0
		4*A10+2*A31+2*A12					[199]
$C_6H_6O_2$		1,2-dihydroxybenzene					
	376.9	22.01	0	58.39	55.2	22.01	20.8
		4*A10+2*A31+2*A12					[199]
$C_6H_6O_2$		1,3-dihydroxybenzene					
	366.8	1.2	3.27				
	382.6	18.9	49.41	52.64	55.2	20.1	21.1
		4*A10+2*A31+2*A12					[199]
$C_6H_6O_3$		1,2,3-trihydroxybenzene					
	407.2	18.55	0	45.56	60.6	18.55	24.7
		3*A10+3*A12+3*A31					[4]
C_6H_6S		thiophenol					
	258.3	11.4	0	44.3	52.6	11.3	13.6
		5*A10+A12+A86					[281]
C_6H_7N		aniline					

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)
	267.1	10.54	0	39.45	51.0	10.54	14.1
		5*A10+A12+A45					[216]
C_6H_7N		2-methylpyridine					
	206.5	9.72	0	47.1	48.5	9.72	10.0
		4*A10+A11+A1+A41					[216]
C_6H_7N		3-methylpyridine					
	255	14.18	0	55.62	48.5	14.18	12.4
		4*A10+A11+A1+A41					[216]
C_6H_7NO		*o*-aminophenol					
	447.4	34	0	75.99	56.3	34	25.2
		4*A10+2*A12+A31+A45					[216]
C_6H_7NO		*m*-aminophenol					
	399	22.98	0	57.59	56.3	22.98	22.5
		4*A10+2*A12+A31+A45					[139]
C_6H_7NO		*p*-aminophenol					
	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
		4*A10+2*A12+A31+A45					[216,223]
C_6H_8		1,3-cyclohexadiene					
	161	4.2	0	26.1	38.0	4.2	6.1
		A14+3*A15+4*A18					[216]
C_6H_8		1,4-cyclohexadiene					
	192	0.82	4.25				
	224	5.72	25.51	29.76	38.0	6.53	8.5
		A14+3*A15+4*A18					[216]
$C_6H_8N_2$		*o*-phenylenediamine					
	373.9	23.1	0	61.78	57.43	23.1	21.47
		4*A10+2*A12+2*A45					[216]
$C_6H_8N_2$		*m*-phenylenediamine					
	335.5	15.4	0	45.9	57.43	15.4	19.27
		4*A10+2*A12+2*A45					[216]
$C_6H_8N_2$		*p*-phenylenediamine					
	412.3	21.7	0	52.63	57.43	21.7	23.68
		4*A10+2*A12+2*A45					[216]
$C_6H_8N_2$		phenylhydrazine					
	292.8	16.43	0	56.11	45.7	16.43	13.4
		5*A10+A12+A45+A44					[215]
$C_6H_8N_2O_2$		N-acetylglycine amide					
	408.2	25.6	0	62.71	54.1	25.6	22.1
		A1+A60+A2+A61					[278]
$C_6H_8N_2O_2$		1,3-dimethyluracil					
	398	14.6	0	36.68	30.0	14.6	11.9
		2*A1+A14+3*A15+2*A125+2*A18*B18					[292]
$C_6H_8N_4O_2$		*bis*(2-cyanoethyl)-N-nitroamine					
	327	44.99	0	137.57	109.1	44.99	35.7
		4*A2+2*A56+A51+A47					[225]
$C_6H_8O_2$		1,4-cyclohexanedione					
	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
		3*A15+A14+2*A114					[114]
$C_6H_8O_4$		dimethyl maleate					
	254	14.64	0	57.74	58.4	14.64	14.8
		2*A1+2*B6*A6+2*A38					[216]
$C_6H_8O_4$		dimethyl fumarate					
	375	35.15	0	93.72	58.4	35.15	21.9
		2*A1+2*A38+2*B6*A6					[216]
$C_6H_8O_4$		DL 3,6-dimethyl-1,4-dioxane-2,5-dione					
	397.5	24.7	0	62.14	49.1	24.7	19.5
		A14+A15+2*A115+2*A16+2*A1					[216]
C_6H_8S		2,5-dimethylthiophene					
	210.6	8.91	0	42.31	51.1	8.91	10.8
		2*A1+A131+A14+2*A15+2*A19+2*A18					[216]
$C_6H_8ClO_2$		chloroethyl methacrylate					
	235.1	17	0	72.31	62.3	17	14.7
		2*A2+A22*B22+A5+A7+A1+A38					[216]
C_6H_9N		2,4-dimethylpyrrole					
	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)	
		$A14+2*A15+A18+2*A1+A121+A18*B18+2*A19$						[70]
C_6H_9N		2,5-dimethylpyrrole						
	280.9	9.3	0	33.09	50.4	9.3	14.2	
		$A14+2*A15+2*A18+2*A1+A121+2*A19$						[216]
C_6H_9NS		2,4,5-trimethylthiazole						
	240.7	9	0	37.39	60.2	9	14.5	
		$A14+2*A15+3*A19+3*A1+A118+A131$						[61]
C_6H_{10}		cyclohexane						
	138.7	4.23	30.5					
	169.7	3.28	19.35	49.85	41.3	7.51	7.0	
		$A14+3*A15+2*A18$						[216]
$C_6H_{10}N_2O$		2,3-diazabicyclo[2.2.2]oct-2-ene N-oxide						
	359.3	5.02	13.97					
	399.3	8.05	20.16					
	438	3.84	8.77	42.9	47.6	16.91	20.8	
		$2*A14+2*A15+2*A16+A123$						[42]
$C_6H_{10}O$		cyclohexanone						
	220.8	8.66	39.22					
	245.2	1.33	5.42	44.64	43.1	9.99	10.6	
		$A14+3*A15+A114$						[156]
$C_6H_{10}O$		cyclohexene oxide						
	193.1	9.54	49.38					
	238.1	1.06	4.47	53.85	42.2	10.6	10.1	
		$2*A14+A15+A112+2*A16$						[156]
$C_6H_{10}O_2$		ε-caprolactone						
	272	13.82	50.81	50.79	51.3	13.82	14.0	
		$A14+4*A15+A115$						[32]
$C_6H_{10}O_3$		2,2-dimethyltrimethylene carbonate						
	324.1	10.3	31.78					
	387.2	5.62	14.52	46.31	46.3	15.92	17.9	
		$A14+3*A15+A116+2*A1+A17$						[200]
$C_6H_{10}O_4$		adipic acid						
	426.4	34.85	0	81.73	69.6	34.85	29.7	
		$4*A2*B2+2*A36*B36$						[340]
$C_6H_{10}O_6$		(*dl*) dimethyl tartrate						
	360.2	26.94	0	74.81	76.7	26.94	27.6	
		$2*A38+2*A3*B3+2*A1+2*A30*D30$						[220]
$C_6H_{10}O_6$		(*d*) dimethyl tartrate						
	322.2	17.36	0	53.89	76.7	17.36	24.7	
		$2*A38+2*A3*B3+2*A1+2*A30*D30$						[220]
$C_6H_{11}Br$		bromocyclohexane						
	216.9	10.79	0	49.75	47.3	10.79	10.3	
		$A14+3*A15+A21+A16$						[190]
$C_6H_{11}Cl$		chlorocyclohexane						
	120	0.05	0.42					
	220.4	8.01	36.35					
	229.3	2.04	8.91	45.67	40.5	10.1	9.3	
		$A14+3*A15+A16+A22$						[229]
$C_6H_{11}NO$		cyclohexanone oxime						
	240.8	0.01	0.06					
	362.6	12.7	35.02					
	273.4	0.09	0.34	35.43	45.8	12.81	12.5	
		$A14+3*A15+A19+A53$						[5]
$C_6H_{11}NO$		*e*-caprolactam						
	343.3	16.1	0	46.89	50.9	16.1	17.5	
		$A14+4*A15+A124$						[6]
$C_6H_{11}NO_3$		N-dimethylaminosuccinamic acid						
	431.4	36.97	0	85.71	54.4	36.97	23.5	
		$2*A1+2*A2+A36*B36+A59$						[221]
$C_6H_{11}N_2O_3PS_2$		S-2,3-dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl O,O-dimethyl phosphorodithioate						
	315.1	28.54	0	90.59	90.7	28.54	28.6	
		$3*A1+A14+2*A15+A138+A19+A118+A32+A80$						[221]
C_6H_{12}		cyclohexane						
	186.1	6.74	36.2					
	279.8	2.68	9.57	45.77	44.5	9.41	12.5	
		$A14+3*A15$						[216]
C_6H_{12}		methylcyclopentane						
	130.7	6.93	0	53.01	43.6	6.93	5.7	
		$A14+A16+A1+2*A15$						[216]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
C_6H_{12}		1-hexene					
	133.4	9.35	0	70.1	61.6	9.37	8.2
		$A1+3*A2+A5+A6$					[216]
C_6H_{12}		2,3-dimethyl-2-butene					
	196.8	3.53	17.94				
	198.9	6.44	32.39	50.34	48.9	9.97	9.6
		$4*A1+2*A7$					[216]
C_6H_{12}		3,3-dimethyl-1-butene					
	124.9	4.35	34.84				
	158.4	1.09	6.87	41.71	40.5	5.44	5.1
		$A4+3*A1+A5+A6$					[216]
C_6H_{12}		*cis*-2-hexene					
	132	8.88	0	67.27	59.9	8.88	7.9
		$2*A1+2*A2+2*A6$					[165]
$C_6H_{12}N_2$		1,4-diazabicyclo[2.2.2]octane					
	351.1	10.54	30.08				
	433	7.45	17.15	47.24	35.6	18.0	15.4
		$2*A14+2*A15+2*A119$					[216]
$C_6H_{12}N_2O_3$		β-alanyl-β-alanine					
	480.1	58.3	0	121.45	81.4	58.3	39.1
		$4*A2+A45+A36*C36+A60$					[216]
$C_6H_{12}N_2O_3$		α-alanyl-α-alanine (DL)					
	483.2	33.2	0	68.72	68.4	33.2	33.0
		$2*A1+A45+A36*C36+A60+2*A3*B3$					[216]
$C_6H_{12}O$		cyclohexanol					
	265.5	8.8	33.3				
	299.1	1.8	6.0	39.3	31.5	9.9	9.4
		$A14+3*A15+A16+A30$					[81]
$C_6H_{12}O$		1-methylcyclopentanol					
	310.2	8.41	0	27.11	25.5	8.41	7.9
		$A14+2*A15+A1+A17+A30$					[230]
$C_6H_{12}O$		hexanal					
	214.9	13.3	61.89				
	243.2	0.34	1.38	63.27	76.4	13.64	18.6
		$A14+4*A2*B2+A34$					[128, 168]
$C_6H_{12}O$		3,3-dimethyl-2-butanone					
	221.7	11.34	0	51.04	52.0	11.34	11.5
		$4*A1+A4*B4+A35$					[216]
$C_6H_{12}O$		3-hexanone					
	145	0.68	4.7				
	217.7	13.47	61.89	66.61	61.1	14.15	13.3
		$2*A1+3*A2+A35$					[216]
$C_6H_{12}O$		2-hexanone					
	217.7	14.9	68.42	68.41	61.1	14.9	13.3
		$2*A1+3*A2+A35$					[216]
$C_6H_{12}O_2$		2,2-dimethyl-1,3-dioxane					
	229.6	12.1	0	52.7	47.5	12.1	10.9
		$A14+3*A15+2*A1+A17+2*A112$					[47]
$C_6H_{12}O_2$		*cis*-1,2-cyclohexanediol					
	360.4	19.89	55.19				
	371.6	3.32	8.93	64.12	51.2	23.21	19.0
		$A14+3*A15+2*A30*B30+2*A16$					[204]
$C_6H_{12}O_2$		*trans*-1,2-cyclohexanediol					
	372.3	18.51	0	49.72	51.2	18.51	19.1
		$A14+3*A15+2*A30*B30+2*A16$					[204]
$C_6H_{12}O_3$		2,4,6-trimethyl-1,3,5-trioxane					
	142.7	0.26	1.81				
	147.5	0.77	5.24				
	285.7	13.52	47.32	54.37	56.7	14.55	16.2
		$3*A1+3*A16+A14+3*A15+3*A112$					[216]
$C_6H_{12}O_6$		α-D-glucose					
	414	31.42	0	75.9	93.0	31.42	38.5
		$A14+3*A15+5*A30*F30+A2+5*A16+A112$					[216]
$C_6H_{12}O_6$		myo-inositol					
	496.9	47.9	0	96.4	92.7	47.9	46.1
		$A14+3*A15+6*A16+6*A30*F30$					[216]
$C_6H_{12}S$		cyclopentyl methyl sulfide					
	165	0.9	5.44				
	169.9	9.2	54.31	59.75	45.7	10.1	7.8
		$A14+2*A15+A1+A84+A16$					[105]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_6H_{12}S$		cyclohexanethiol					
	189.6	10	0	52.72	52.8	10.0	10.0
		$A14+3*A15+A86+A16$					[341]
$C_6H_{13}Br$		1-bromohexane					
	188.1	18.05	0	95.98	81.8	18.05	15.4
		$A1+5*A2*B2+A21$					[216]
$C_6H_{13}N$		2-methylpiperidine					
	269.4	18.58	0	68.99	49.5	18.58	13.3
		$A14+3*A15+A121+A1+A16$					[216]
$C_6H_{13}NO$		hexanamide					
	374	25.1	0	67.12	82.8	25.1	31.0
		$4*A2*B2+A1+A61$					[279]
C_6H_{14}		*n*-hexane					
	177.8	13.08	0	73.22	72.5	13.08	12.9
		$2*A1+4*A2*B2$					[216]
C_6H_{14}		2,3-dimethylbutane					
	136.1	6.43	47.22				
	107	2.37	22.13				
	145.2	0.79	5.47	52.96	37.6	9.59	5.1
		$4*A1+2*A3$					[216]
C_6H_{14}		3-methylpentane					
	110.3	5.31	0	48.17	50.6	5.31	5.6
		$2*A2+3*A1+A3$					[216]
C_6H_{14}		2-methylpentane					
	119.6	6.27	0	52.43	50.6	6.27	6.05
		$2*A2+3*A1+A3$					[216]
C_6H_{14}		2,2-dimethylbutane					
	126.8	5.4	42.57				
	140.8	0.28	2.02				
	174.3	0.58	3.31	45.88	42.6	6.26	7.4
		$4*A1+A2+A4$					[216]
$C_6H_{14}O$		1-hexanol					
	225.8	15.48	0	68.56	66.0	15.48	14.9
		$A1+5*A2*B2+A30$					[216]
$C_6H_{14}O$		isopropyl ether					
	187.8	12.05	0	64.02	55.7	12.05	10.5
		$4*A1+2*A3*B3+A32$					[66]
$C_6H_{14}O$		4-oxaheptane					
	158.4	10.77	0	67.99	68.4	10.77	10.8
		$2*A1+4*A2+A32$					[216]
$C_6H_{14}O_2$		2,3-dimethyl-2,3-butanediol					
	316.2	14.7	0	46.49	60.8	14.7	19.2
		$4*A1+2*A4*B4+2*B30*A30$					[231]
$C_6H_{14}O_2$		1,6-hexanediol					
	320.6	25.52	0	79.6	92.2	25.52	29.0
		$2*A30*B30+6*A2*B2$					[216]
$C_6H_{14}O_3$		2,5,8-trioxanonane					
	209.1	17.8	0	85.1	77.8	17.8	16.3
		$2*A1+4*A2+3*A32$					[216]
$C_6H_{14}O_6$		D sorbitol					
	366.5	30.2	0	82.4	111.7	30.2	40.9
		$2*A2+4*A3*B3+6*A30*F30$					[216]
$C_6H_{14}O_6$		dulcitol					
	460.3	65.1	0	141.4	111.7	65.1	51.4
		$2*A2+4*A3*B3+6*A30*F30$					[216]
$C_6H_{14}O_6$		D mannitol					
	439.1	56.1	0	127.8	111.7	56.1	49.0
	438.7	50.6	0	115.3	111.7	50.6	49.0
		$2*A2+4*A3*B3+6*A30*F30$					[216, 394]
$C_6H_{14}S$		diisopropyl sulfide					
	195.1	10.42	0	53.39	52.8	10.42	10.4
		$4*A1+2*A3*B3+A84$					[341]
$C_6H_{14}S$		dipropyl sulfide					
	170.4	12.14	0	71.25	65.8	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_6H_{14}S$		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_{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)
	503.8	32.23	0	63.97	73.1	32.23	36.8
		3*A29+A36*D36+4*A12+2*A10					[215]
$C_7H_4Cl_2O_2$		3,5-dichlorobenzoic acid					
	459.3	22.97	0	50.01	62.2	22.97	28.6
		3*A12+3*A10+2*A22*C22+A36*C36					[215]
$C_7H_4Cl_3NO_3$		3,5,6-trichloro-2-pyridinyloxyacetic acid					
	423.3	31.17	0	73.63	78.8	31.17	33.4
		A10+4*A12+3*A22*F22+A41+A32+A36*F36+A2					[221]
$C_7H_4N_2O_6$		3,5-dinitrobenzoic acid					
	480.4	22.8	0	47.47	65.3	22.8	31.4
		3*A12+2*A50+A36*C36+3*A10					[280]
$C_7H_5Cl_3N_2O_2$		methyl 4-amino-3,5,6-trichloro-2-picolinate					
	394.3	26.78	0	67.91	68.7	26.78	27.1
		5*A12+A41+A38+3*A22*F22+A45+A1					[232]
$C_7H_5ClO_2$		2-chlorobenzoic acid					
	413.4	25.73	0	62.34	47.0	25.73	19.4
		4*A10+A36*B36+2*A12+A22*B22					[215]
$C_7H_5ClO_2$		3-chlorobenzoic acid					
	427.4	23.85	0	55.65	47.0	23.85	20.1
		4*A10+A36*B36+2*A12+A22*B22					[215]
$C_7H_5ClO_2$		4-chlorobenzoic acid					
	512.9	32.26	0	62.76	47.0	32.26	24.1
		4*A10+A36*B36+2*A12+A22*B22					[215]
$C_7H_5Cl_2NO_2$		3-amino-2,5-dichlorobenzoic acid					
	475.6	37.42	0	78.68	68.7	37.42	32.7
		2*A22*D22+A45+A36*D36+4*A12+2*A10					[215]
$C_7H_5Cl_3$		benzotrichloride					
	236.0	13.95	0	59.11	53.2	13.95	12.6
		5*A10+A11+3*A22*C22+A4*B4					[216]
$C_7H_5F_3$		benzotrifluoride					
	244.1	13.78	0	56.45	44.7	13.77	10.9
		5*A10+A11+A4*B4+3*A25					[216]
$C_7H_5IO_2$		2-iodobenzoic acid					
	435.1	21.38	0	49.14	50.2	21.38	21.8
		4*A10+2*A12+A36*B36+A29					[7]
$C_7H_5IO_2$		3-iodobenzoic acid					
	460.4	28.7	0	62.34	50.2	28.7	23.1
		4*A10+2*A12+A36*B36+A29					[7]
$C_7H_5IO_2$		4-iodobenzoic acid					
	543.8	35.24	0	64.8	50.2	35.24	27.3
		4*A10+2*A12+A36*B36+A29					[7]
C_7H_5N		benzonitrile					
	260.3	10.98	0	42.18	47.3	10.98	12.3
		5*A10+A12+A56					[134]
C_7H_5NO		benzoxazole					
	247	0.02	0.07				
	302.5	16.78	55.48	55.56	44.6	16.8	13.5
		A14+2*A15+2*A19+A18*B18+A112+A118+4*A10					[216]
$C_7H_5NO_4$		*o*-nitrobenzoic acid					
	419	27.99	0	66.8	48.5	27.99	20.3
		4*A10+2*A12+A36*B36+A50					[216]
$C_7H_5NO_4$		*m*-nitrobenzoic acid					
	414.3	19.33	0	46.66	48.5	19.33	20.1
		4*A10+2*A12+A50+A36*B36					[216]
$C_7H_5NO_4$		*p*-nitrobenzoic acid					
	512.4	36.9	0	72.02	48.5	36.9	24.9
		4*A10+2*A12+A36*B36+A50					[215]
C_7H_5NS		benzothiazole					
	275.6	12.8	0	46.36	46.2	12.8	12.7
		4*A10+A14+2*A15+A118*+2*A19+A131+A18*B18					[216]
$C_7H_5N_3O_6$		2,4,5-trinitrotoluene					
	376.2	24.7	0	66.0	53.5	24.7	20.1
		2*A10+3*A12+3*A50*C50+A1+A11					[216]
$C_7H_5N_3O_6$		2,4,6-trinitrotoluene					
	352.2	23.43	0	66.52	53.5	23.43	18.9
		2*A10+3*A12+3*A50*C50+A1+A11					[217]
$C_7H_5N_5O_8$		N-methyl-2,4,6,N-tetranitroaniline					
	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_7H_6N_2$		benzimidazole					
	443.2	19.25	0	43.43	45.5	19.25	20.2
		4*A10+A118+A121+A14+2*A15+2*A19+A18*B18					[282]
$C_7H_6N_2O_4$		2,4-dinitrotoluene					
	343.3	20.12	0	58.61	50.7	20.12	17.4
		3*A10+A11+2*A12+2*A50+A1					[215]
$C_7H_6N_2O_4$		2,6-dinitrotoluene					
	327.5	23.85	0	72.82	50.7	23.85	16.6
		3*A10+A11+2*A12+2*A50+A1					[217]
$C_7H_6N_2O_4$		2,3-dinitrotoluene					
	329.8	17.57	0	53.27	50.7	17.57	16.7
		3*A10+A11+2*A12+2*A50+A1					[217]
$C_7H_6N_2O_4$		3,4-dinitrotoluene					
	329.5	18.83	0	57.15	50.7	18.83	16.7
		3*A10+A11+2*A12+2*A50+A1					[217]
$C_7H_6N_2O_5$		2-methyl-4,6-dinitrophenol					
	359.3	19.41	0	54.02	56.1	19.41	20.2
		3*A12+A11+2*A10+A1+A31+2*A50					[215]
C_7H_6O		benzaldehyde					
	216	9.32	0	43.1	51.1	9.32	11.0
		5*A10+A12+A34					[216]
$C_7H_6O_2$		benzoic acid					
	395.5	18.0	0	45.45	43.0	18.0	17.0
		5*A10+A12+A36					[282]
$C_7H_6O_3$		2-hydroxybenzoic acid					
	431.8	24.6	0	56.97	51.1	24.6	22.1
		4*A10+2*A12+A31+A36*B36					[216,8]
$C_7H_6O_3$		3-hydroxybenzoic acid					
	475.1	26.2	0	55.15	51.1	26.2	24.3
		4*A10+2*A12+A31+A36*B36					[216,8]
$C_7H_6O_3$		4-hydroxybenzoic acid					
	488.1	30.9	0	63.31	51.1	30.9	24.9
		4*A10+2*A12+A31+A36*B36					[233]
C_7H_7Br		benzylbromide					
	271.8	13.2	0	48.57	52.2	13.2	14.2
		5*A10+A11+A2+A21					[49]
C_7H_7Br		4-bromotoluene					
	301.2	15.13	0	50.2	47.1	15.1	14.3
		4*A10+A11+A12+A1+A21					[234]
C_7H_7Cl		*p*-chlorotoluene					
	280.7	13.55	0	48.29	40.9	13.55	11.5
		A1+A12+A11+4*A10+A22					[234]
$C_7H_7ClN_2S$		1-(*o*-chlorophenyl)thiourea					
	413.5	22.29	0	53.91	53.9	22.29	22.3
		4*A10+2*A12+A22*B22+A91					[221]
C_7H_7F		2-fluorotoluene					
	210.7	9.8	0	46.51	46.8	9.8	9.9
		4*A10+A11+A12+A1+A24					[216]
C_7H_7F		3-fluorotoluene					
	184	8.3	0	45.11	46.8	8.3	8.6
		4*A10+A11+A12+A1+A24					[216]
C_7H_7F		4-fluorotoluene					
	216.5	9.35	0	43.18	46.8	9.35	10.13
		4*A10+A11+A1+A12+A24					[216]
C_7H_7I		benzyliodide					
	299.5	13.2	0	44.07	54.0	13.2	16.2
		5*A10+A11+A2+A29					[46]
C_7H_7I		*p*-iodotoluene					
	306.7	14.96	0	48.79	49.5	14.96	15.2
		4*A10+A11+A12+A29+A1					[234]
C_7H_7NO		benzamide					
	402.3	18.49	0	45.96	57.5	18.49	23.1
		5*A10+A12+A61					[215]
$C_7H_7NO_2$		3-nitrotoluene					
	370	19.2	0	51.88	47.9	19.2	17.7
		4*A10+A1+A11+A12+A50					[235]
$C_7H_7NO_2$		4-nitrotoluene					

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)
	318	16.9	53.1				
	324.8	16.81	0	51.76	47.9	16.81	15.6
		4*A10+A12+A11+A1+A50					[215]
$C_7H_7NO_2$		2-aminobenzoic acid					
	417.8	20.5	0	49.07	52.2	20.5	21.8
		4*A10+2*A12+A36*B36+A45					[215]
$C_7H_7NO_2$		3-aminobenzoic acid					
	452.9	21.84	0	48.12	52.2	21.84	23.6
		4*A10+2*A12+A36*B36+A45					[215]
$C_7H_7NO_2$		4-aminobenzoic acid					
	461.4	20.92	0	45.19	52.2	20.92	24.1
		4*A10+2*A12+A36*B36+A45					[215]
$C_7H_7NO_3$		4-nitro-5-methylphenol					
	401	27.4	0	68.33	53.3	27.4	21.4
		3*A10+A1+A11+2*A12+A31+A50					[215]
$C_7H_7NO_3$		2-nitro-5-methylphenol					
	302.8	20.79	0	68.66	53.3	20.79	16.1
		3*A10+A1+A11+2*A12+A31+A50					[215]
$C_7H_7N_3O_2$		N-acetyl-pyrazinamide					
	366.7	23.6	0	64.36	61.9	23.6	22.7
		3*A10+A12+2*A41+A71+A1					[9]
C_7H_8		toluene					
	178.0	6.62	0	37.15	45.0	6.62	8.0
		5*A10+A1+A11					[216]
C_7H_8		cycloheptatriene					
	154.0	2.35	15.24				
	198.0	1.16	5.86	21.11	38.5	3.51	7.6
		A14+4*A15+6*A18					[216]
C_7H_8		tetracyclo[3.2.0.0(2,7).0(4,6)]heptane					
	180	7.2	40				
	228	1.09	4.8	44.8	26.6	8.29	6.1
		4*A14−5*A15+6*A16					[216]
$C_7H_8N_2O$		phenylurea					
	420.6	23.68	0	56.3	52.1	23.68	21.9
		5*A10+A12+A67					[215]
$C_7H_8N_4O_2$		theophylline					
	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
		2*A14+3*A15+2*A125+A118+A121+2*A1+2*A19+A18*B18					[236,205]
C_7H_8O		benzyl alcohol					
	257.6	8.79	0	34.11	36.4	8.79	9.4
		5*A10+A11+A2+A30					[215]
C_7H_8O		*o*-hydroxytoluene					
	304.2	15.82	0	52.01	50.4	15.82	15.3
		A31+A1+A12+4*A10+A11					[216]
C_7H_8O		*m*-hydroxytoluene					
	285.4	10.71	0	37.53	50.42	10.71	14.39
		A31+A1+A12+4*A10+A11					[216]
C_7H_8O		*p*-hydroxytoluene					
	307.9	12.72	0	41.25	50.42	12.72	15.52
		A31+A1+A12+4*A10+A11					[216]
C_7H_8O		methoxybenzene					
	268.7	12.9	0	48.0	51.9	12.9	13.9
		5*A10+A12+A1+A32					[216]
C_7H_8S		methylphenylsulfide					
	256.4	14.85	0	57.86	49.3	14.85	12.63
		5*A10+A12+A1+A84					[105]
$C_7H_9Cl_3NO_3PS$		O,O-dimethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate					
	318.7	25.92	0	81.32	73.2	25.92	23.3
		4*A12+A10+A41+3*A22*E22+2*A1+A79					[221]
$C_9H_{13}Cl_3NO_4P$		O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphate					
	312.5	15.61	0	49.97	76.4	15.61	23.9
		4*A12+A10+A41+3*A22*E22+2*A1+A74+2*A2					[221]
C_7H_9N		*m*-toluidine					
	241.7	8.8	0	36.41	51.5	8.8	12.5
		A45+4*A10+A12+A1+A11					[215]
C_7H_9N		*p*-toluidine					
	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
C_7H_9N		*o*-toluidine					
	249.6	8.08	0	32.37	51.5	8.08	12.9
		*A*45+4**A*10+*A*12+*A*1+*A*11					[215]
C_7H_9N		2-methylaniline					
	258	11.66	0	45.1	51.5	11.66	14.8
		4**A*10+*A*11+*A*12+*A*1+*A*45					[30]
C_7H_9N		2,3-dimethylpyridine					
	258.6	13.48	0	52.13	49.1	13.48	12.7
		2**A*1+2**A*11+3**A*10+*A*41					[69]
C_7H_9N		2,4-dimethylpyridine					
	209.4	8.82	0	42.12	49.1	8.82	10.3
		2**A*1+2**A*11+3**A*10+*A*41					[69]
C_7H_9N		2,5-dimethylpyridine					
	259.1	14.64	0	56.5	49.1	14.64	12.7
		2**A*1+2**A*11+3**A*10+*A*41					[69]
C_7H_9N		2,6-dimethylpyridine					
	267.1	13.04	0	48.82	49.1	13.04	13.1
		2**A*1+2**A*11+3**A*10+*A*41					[69]
C_7H_9N		3,4-dimethylpyridine					
	262.7	14.7	0	55.96	49.1	14.7	12.9
		2**A*1+2**A*11+3**A*10+*A*41					[69]
C_7H_9N		3,5-dimethylpyridine					
	266.9	13.11	0	49.12	49.1	13.11	13.1
		2**A*1+2**A*11+3**A*10+*A*41					[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**A*4**B*4+3**A*2+*A*1+5**A*50+*A*38					[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**A*4**B*4+3**A*2+*A*1+5**A*50+*A*38					[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**A*14+*A*15+2**A*16+2**A*18					[129,349]
$C_7H_{10}O$		2-norbornanone					
	368.7	3.39	0	9.19	39.7	3.39	14.6
		2**A*14+*A*15+2**A*16+*A*114					[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**A*14+2**A*16+2**A*16+*A*123					[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**A*1+*A*60+*A*3**B*3+*A*61					[278]
$C_7H_{10}N_2O_2$		1,3,6-trimethyluracil					
	384.5	21.2	0	55.14	38.4	21.2	14.8
		*A*14+3**A*15+2**A*125+3**A*1+*A*18**B*18+*A*19					[216]
$C_7H_{10}O_3$		3,3-dimethylpentanedioic anhydride					
	396.2	17.99	0	45.41	47.4	17.99	18.8
		*A*14+3**A*15+2**A*1+*A*17+*A*117					[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
		*A*14+3**A*15+*A*16+*A*56					[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
		*A*14+3**A*15+*A*16+*A*57					[216]
C_7H_{12}		4-methylcyclohex-1-ene					
	153.6	6.63	0	43.16	44.1	6.63	6.77
		*A*14+3**A*15+*A*1+*A*16+2**A*18					[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
		*A*14+4**A*15+2**A*18					[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_{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)
		3*A41+A22*F22+3*A12+2*A44+2*A1+2*A2					[221]
$C_7H_{12}O_2$		butyl acrylate					
	209.5	17.31	0	82.61	67.9	17.31	14.2
		A1+3*A2+A38+A5+A6*B6					[216]
$C_7H_{12}O_4$		pimilic acid					
	377.5	27.62	0	73.17	78.9	27.62	29.8
		5*A2*B2+2*A36*B36					[340]
$C_7H_{12}O_4S_2$		(*dl*) methylenebisthiopropionic acid					
	429	39.33	0	91.68	86.9	39.33	37.3
		2*A36*D36+2*A84+2*A3*B3+2*A1+A2					[273]
$C_7H_{12}O_4S_2$		(*d*) methylenebisthiopropionic acid					
	355	22.59	0	63.64	86.9	22.59	30.8
		2*A36*D36+2*A84+2*A3*B3+2*A1+A2					[273]
$C_7H_{13}N$		1-azabicyclo[2.2.2]octane					
	196	5.23	26.53				
	430	5.86	13.81	40.33	40.1	11.09	17.3
		2*A14+2*A15+A16+A119					[216]
$C_7H_{13}NO$		ζ-enantholactam					
	310.3	13.78	0	44.39	54.6	13.78	16.9
		A14+5*A15+A124					[216]
$C_7H_{13}N_3O_3S$		N,N-dimethyl-2-methylcarbamoyloxyimino-2-(methylthio)acetamide					
	372.2	30.17	0	81.04	59.4	30.17	22.1
		4*A1+A59+A7+A42+A69+A84					[221]
C_7H_{14}		cycloheptane					
	134.8	4.98	36.94				
	198.2	0.29	1.46				
	212.4	0.45	2.11				
	265.1	1.88	7.1	47.6	48.2	7.6	12.8
		4*A15+A14					[216]
C_7H_{14}		1,1-dimethylcyclopentane					
	146.8	6.49	44.18				
	203.7	1.09	5.34	49.52	41.4	7.57	8.4
		A14+A17+2*A1+2*A15					[216]
C_7H_{14}		*cis*-1,2-dimethylcyclopentane					
	141.5	6.65	47.01				
	219.4	1.66	7.55	54.57	46.5	8.31	10.2
		A14+2*A16+2*A1+2*A15					[216]
C_7H_{14}		*trans*-1,3-dimethylcyclopentane					
	139.5	7.4	0	53.09	46.5	7.4	6.5
		A14+2*A16+2*A1+2*A15					[216]
C_7H_{14}		ethylcyclopentane					
	134.7	6.87	0	51.0	50.8	6.87	6.8
		A14+A16+A1+A2+2*A15					[216]
C_7H_{14}		methylcyclohexane					
	146.6	6.75	0	46.1	47.3	6.75	6.9
		A14+A16+A1+3*A15					[216]
C_7H_{14}		1-heptene					
	154.3	12.66	0	82.5	77.5	12.66	12.0
		A1+4*A2*B2+A5+A6					[216]
$C_7H_{14}NO_5P$		dimethyl(E)-1-methyl-2-methylcarbamoylvinyl phosphate					
	326.9	22.36	0	68.4	55.0	22.36	18.0
		4*A1+A7+A6*B6+A60+A74					[221]
$C_7H_{14}N_2O_2S$		2-methyl-2(methylythio)propionaldehyde O-methylcarbamoyloxime					
	374.0	22.71	0	60.73	62.3	22.71	23.3
		4*A1+A4*B4+A6*B6+A69+A84+A42					[221]
$C_7H_{13}N_3O_3S$		N,N-dimethyl-2-methylcarbamoyloxyimino-2-(methylthio)acetamide					
	372.2	30.17	0	81.05	59.4	30.17	22.1
		4*A1+A59+A7+A84+A42+A69					[221]
$C_7H_{14}O$		heptanal					
	229.3	22.89	0	99.83	85.8	22.89	19.7
		A1+5*A2*B2+A34					[43]
$C_7H_{14}O$		diisopropyl ketone					
	204.8	11.2	0	54.6	55.3	11.2	11.3
		4*A1+2*A3*B3+A35					[216]
$C_7H_{14}O$		1-methylcyclohexanol					
	299.2	10.87	0	36.34	29.2	10.87	8.8
		A14+3*A15+A1+A17+A30					[230]
$C_7H_{14}O$		cycloheptanol					
	172.2	2.93	16.98				

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)
	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
		$A14+4*A15+A30+A16$					[216]
$C_7H_{14}O_2$		heptanoic acid					
	224.8	2.04	9.08				
	265.8	15.44	58.07	67.15	77.6	17.48	20.6
		$5*A2*B2+A1+A36$					[216,143]
$C_7H_{15}Cl_2N_2O_2P$		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
		$A14+3*A15+A144+4*A2+2*A22*C22$					[221]
C_7H_{16}		heptane					
	182.6	14.04	0	76.9	81.8	14.04	14.9
		$2*A1+5*A2*B2$					[216]
C_7H_{16}		2,4-dimethylpentane					
	154.0	6.85	0	44.46	44.7	6.85	6.9
		$4*A1+A2+2*A3$					[216]
C_7H_{16}		3-ethylpentane					
	154.6	9.55	0	61.77	57.8	9.55	8.9
		$3*A1+3*A2+A3$					[216]
C_7H_{16}		2-methylhexane					
	154.9	9.18	0	59.29	57.8	9.18	9.0
		$3*A1+3*A2+A3$					[216]
C_7H_{16}		3,3-dimethylpentane					
	138.2	7.07	0	51.16	49.7	7.07	6.9
		$4*A1+A4+2*A2$					[216]
C_7H_{16}		2,2,3-trimethylbutane					
	121	2.38	19.64				
	247.7	2.2	8.88	28.53	36.7	4.58	4.4
		$5*A1+A3+A4$					[216]
C_7H_{16}		2,2-dimethylpentane					
	148.1	5.86	0	39.55	49.74	5.86	7.37
		$4*A1+A4+2*A2$					[215]
$C_7H_{16}O$		1-heptanol					
	240.4	18.16	0	75.53	75.31	18.16	18.1
		$A1+6*A2*B2+A30$					[216]
$C_7H_{16}O_2$		1,7-heptanediol					
	295.2	21.3	0	72.15	101.6	21.3	30.0
		$7*A2*B2+2*A30*B30$					[215]
$C_7H_{16}S$		1-heptanethiol					
	229.9	25.4	0	110.4	96.6	25.4	22.2
		$A1+6*A2*B2+A86$					[216]
$C_7H_{17}NSi$		N-(β-trimethylsilyethyl)ethylenimine					
	176.5	10.62	0	60.17	54.0	10.62	9.5
		$3*A1+2*A2+A14+A119+A109$					[216]
$C_7H_{20}Si_2$		hexamethyldisilylmethane					
	140.7	11.11	0	78.98	58.5	11.11	8.2
		$6*A1+2*A109+A2$					[216]
$C_8Cl_4N_2$		2,4,5,6-tetrachloro-1,3-benzenedicarbonitile					
	526.2	30	0	57.01	55.3	30	29.1
		$4*A22*F22+2*A56+6*A12$					[221]
C_8F_{18}		perfluorooctane					
	176.5	3.14	17.79				
	254.2	9.58	37.69	55.48	93.8	12.72	23.8
		$8*A4*B4+12*A26+6*A25$					[67]
$C_8H_3NO_5$		3-nitrophthalic anhydride					
	436.2	18.4	0	42.18	51.0	18.4	22.3
		$A14+2*A15+A117+2*A19+A12+3*A10+A50$					[179]
$C_8H_3NO_5$		4-nitrophthalic anhydride					
	388.2	17.14	0	44.15	51.0	17.14	19.8
		$A14+2*A15+A117+2*A19+A12+3*A10+A50$					[179]
$C_8H_4Cl_2O_2$		terephthalyl dichloride					
	337.3	2.34	6.92				
	356.1	21.1	59.25	66.18	66.2	23.44	23.6
		$4*A10+2*A12+2*A40$					[216]
$C_8H_4N_2$		1,2-dicyanobenzene					
	414.1	20	0	48.3	50.2	20	20.8
		$4*A10+2*A12+2*A56$					[71]
$C_8H_4O_3$		phthalic anhydride					
	403.3	23.09	0	57.25	48.2	23.09	19.4
		$A14+2*A15+2*A19+A117+4*A10$					[215]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_8H_5Cl_3O_2$		2,3,6-trichlorophenylacetic acid					
	432.3	22.43	0	51.89	68.5	22.43	29.6
		2*A10+3*A12+A11+A36*D36+3*A22*D22+A2					[215]
$C_8H_5Cl_3O_3$		(2,4,5-trichlorophenoxy)acetic acid					
	431.2	38	0	88.13	75.3	38	32.5
		3*A22*E22+A32+A36*E36+4*A12+2*A10+A2					[215]
$C_8H_5Cl_3O_4$		3,6-dichloro-5-hydroxy-2-methoxybenzoic acid					
	409.9	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					
	228	9.46	0	41.49	41.7	9.46	9.5
		5*A10+A12+A8+A9					[132]
$C_8H_6Cl_2O_3$		(2,4-dichlorophenoxy)acetic acid					
	412.5	35.33	0	85.64	74.0	35.33	30.5
		3*A10+3*A12+A2+2*A22*D22+A36*D36+A32*D32					[221]
$C_8H_6Cl_2O_3$		3,6-dichloro-2-methoxybenzoic acid					
	386.7	22.9	0	59.23	69.6	22.9	26.9
		4*A12+2*A10+2*A22*D22+A36*D36+A32*D32+A1					[215]
$C_8H_6Cl_2O_3$		2,4-dichloro-2-methoxybenzoic acid					
	412.5	35.33	0	85.65	69.6	35.33	28.7
		4*A12+2*A10+2*A22*D22+A36*D36+A32*D32+A1					[215]
$C_8H_6Cl_2O_4$		3,6-dichloro-5-hydroxy-2-methoxybenzoic acid					
	409.8	28.98	0	70.71	75.0	28.98	30.7
		A10+5*A12+2*A22*E22+A36*E36+A1+A32+A31					[215]
$C_8H_6Cl_4$		tetrachloro-*o*-xylene					
	359.2	21.46	0	59.74	50.8	21.46	18.2
		4*A12+2*A11+2*A1+4*A22*D22					[215]
$C_8H_6Cl_4$		tetrachloro-*p*-xylene					
	368.2	22.59	0	61.35	50.8	22.59	18.7
		4*A12+2*A11+2*A1+4*A22*D22					[215]
$C_8H_6Cl_4O_4$		methyl tetrachloroterephthalic acid ester					
	444.3	16.89	0	38.03	92.7	16.89	41.2
		6*A12+2*A1+A38+4*A22*F22+A36					[221]
$C_8H_6N_2$		phthalazine					
	364.5	13.32	0	36.54	51.4	13.32	18.7
		6*A10+2*A12+2*A41					[29]
$C_8H_6N_2$		quinazoline					
	320.9	16.95	0	52.82	51.4	16.95	16.5
		6*A10+2*A12+2*A41					[29]
$C_8H_6N_2$		quinoxaline					
	305.7	11.80	0	38.61	51.4	11.80	15.7
		6*A10+2*A12+2*A41					[29]
$C_8H_6N_2OS_2$		6-methyl-1,3-dithiolo[4,5-*b*]quinoxalin-2-one					
	443.2	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]
C_8H_6S		benzothiophene					
	304.5	11.82	0	38.82	44.1	11.82	13.4
		4*A10+A14+2*A15+A19+A18+A131+A19+A18*B18					[95]
$C_8H_7ClO_3$		(*d*) *o*-chloromandelic acid					
	392.5	24.69	0	62.89	66.1	24.69	25.9
		4*A10+A11+A12+A3*B3+A30*C30+A36*C36+A22*C22					[220]
$C_8H_7ClO_3$		(*dl*) *o*-chloromandelic acid					
	358.5	20.08	0	56.02	66.0	20.08	23.6
		4*A10+A11+A12+A3*B3+A30*C30+A36*C36+A22*C22					[220]
$C_8H_7ClO_3$		(*dl*) *p*-chloromandelic acid					
	394	27.2	0	69.03	66.0	27.2	26.0
		4*A10+A12+A11+A3*B3+A30*C30+A36*C36+A22*C22					[220]
$C_8H_7ClO_3$		(*d*) *p*-chloromandelic acid					
	394	23.01	0	58.41	66.0	23.01	26.0
		4*A10+A11+A12+A3*B3+A30*C30+A36*C36+A22*C22					[220]
$C_8H_7Cl_2NO$		methyl-3,4-dichlorophenylcarbamate					
	381.4	23.19	0	60.8	60.4	23.19	23.0
		A1+3*A10+3*A12+2*A22*C22+A69					[221]
$C_8H_7FO_3$		(*dl*) *m*-fluoromandelic acid					
	370	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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]
$C_8H_7FO_3$		(*d*) *m*-fluoromandelic acid					
	394	24.27	0	61.59	66.4	24.27	26.2
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]
$C_8H_7FO_3$		(*dl*) *o*-fluoromandelic acid					
	390	30.12	0	77.24	66.4	30.12	25.9
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]
$C_8H_7FO_3$		(*d*) *o*-fluoromandelic acid					
	363	20.92	0	57.63	66.4	20.92	24.17
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]
$C_8H_7FO_3$		(*dl*) *p*-fluoromandelic acid					
	403	29.29	0	72.67	66.4	29.29	26.8
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]
$C_8H_7FO_3$		(*d*) *p*-fluoromandelic acid					
	426	30.54	0	71.7	66.4	30.54	28.3
		4*A10+A11+A12+A3*B3+A36*C36+A30*C30+A24					[220,187]
$C_8H_7ClO_3$		4-chlorophenoxyacetic acid					
	429.6	36.27	0	84.42	72.8	36.27	31.3
		4*A10+2*A12+A22*C22+A36*C36+A2+A32					[221]
$C_8H_7N_3O_6$		2,4,6-trinitro-1,3-dimethylbenzene					
	455.4	38.49	0	84.52	54.1	38.49	24.64
		A10+2*A11+3*A12+2*A1+3*A50					[197]
$C_8H_7N_5O_8$		2,4,6,N-tetranitro-N-methyltoluidene					
	375.6	19.33	0	51.46	54.3	19.33	20.4
		4*A12+A10+A11+3*A50+2*A1+A51+A49					[216]
$C_8H_7N_5O_8$		2,4,6-N-tetranitroethylaniline					
	369	23.51	0	63.6	60.8	23.51	22.4
		A51+4*A12+2*A10+A1+A2+3*A50+A49					[216]
C_8H_8		cubane					
	394	5.94	15.08				
	404.9	8.7	21.49	36.56	23.2	14.64	9.4
		5*A14−7*A15+8*A16					[150]
C_8H_8		styrene					
	242.3	10.95	0	45.16	52.2	10.95	12.6
		5*A10+A5+A6+A12					[216]
C_8H_8		cyclooctatetraene					
	268.5	11.27	0	41.49	39.0	11.27	10.5
		A14+5*A15+8*A18					[216]
$C_8H_8BrCl_2O_3PS$		O-(4-bromo-2,5-dichlorophenyl)O,O-dimethyl phosphorothioate					
	325.3	31.15	0	95.74	71.1	31.15	23.1
		2*A10+4*A12+2*A1+2*A22*D22+A21+A79					[221]
$C_8H_8Br_2$		α,α'-dibromo-*o*-xylene					
	368.2	26.78	0	72.73	59.8	26.78	22.0
		4*A10+2*A11+2*A2+2*A21*B21					[215]
$C_8H_8Br_2$		α,α'-dibromo-*m*-xylene					
	350.2	23.69	0	67.65	59.8	23.69	21.0
		4*A10+2*A11+2*A2+2*A21*B21					[215]
$C_8H_8ClNO_2$		N-methyl-2-chlorophenylcarbamic acid ester					
	362.7	21.81	0	60.12	59.1	21.81	21.4
		A1+4*A10+2*A12+A69+A22*B22					[221]
$C_8H_8Cl_2$		α,α'-dichloro-*o*-xylene					
	328.2	21.26	0	64.78	57.1	21.26	18.7
		4*A10+2*A11+2*A2+2*A22*B22					[215]
$C_8H_8Cl_2$		α,α'-dichloro-*m*-xylene					
	307.2	19.51	0	63.51	57.1	19.51	17.5
		4*A10+2*A11+2*A2+2*A22*B22					[215]
$C_8H_8Cl_2$		α,α'-dichloro-*p*-xylene					
	373.2	23.97	0	64.23	57.1	23.97	21.3
		4*A10+2*A11+2*A2+2*A22*B22					[215]
$C_8H_8Cl_2O_2$		1,4-dichloro-2,5-dimethoxybenzene					
	403.9	27.56	0	68.23	61.8	27.56	25.0
		4*A12+2*A10+2*A22*D22+2*A32*D32+2*A1					[215]
$C_8H_8Cl_2O_3$		methyl 3,6-dichloro-2-methoxybenzoate					
	304.6	18.49	0	60.72	64.8	18.49	19.7
		2*A10+4*A12+2*A1+2*A22*D22+A38*D38+A32*D32					[221]
$C_8H_8Cl_3O_3PS$		O,O-dimethyl O-(2,4,5-trichlorophenyl) phosphorothioate					

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)
	313.0	18.94	0	60.51	69.7	18.94	21.8
		2*A10+4*A12+3*A22*D22+2*A1+A79					[221]
$C_8H_8O_2$		*o*-toluic acid					
	376.9	20.17	0	53.51	43.5	20.17	16.4
		4*A10+A12+A11+A1+A36					[215]
$C_8H_8O_2$		*m*-toluic acid					
	381.9	15.73	0	41.19	43.5	15.73	16.6
		4*A10+A12+A11+A1+A36					[215]
$C_8H_8O_2$		*p*-toluic acid					
	452.8	22.72	0	50.17	43.5	22.72	19.7
		4*A10+A12+A11+A1+A36					[215]
$C_8H_8O_2$		phenylacetic acid					
	349.9	14.49	0	41.41	48.0	14.49	16.8
		5*A10+A11+A2+A36					[215]
$C_8H_8O_2$		methyl benzoate					
	261	13.9	0	53.26	54.8	13.9	14.3
		5*A10+A1+A38+A12					[247]
$C_8H_8O_2S$		phenyl vinyl sulfone					
	343.4	11.72	0	34.12	52.5	11.72	18.0
		5*A10+A5+A6+A12+A88					[238]
$C_8H_8O_3$		methyl 4-hydroxybenzoate					
	398.5	24.31	0	61	60.2	24.31	24.0
		4*A10+2*A12+A1+A31+A38*B38					[239]
$C_8H_8O_3$		(*dl*) mandelic acid					
	392	25.52	0	65.11	51.9	25.52	20.3
		5*A10+A3*B3+B30*A30+A36*B36+A11					[220]
$C_8H_8O_3$		(*d*) mandelic acid					
	406	23.36	0	64.92	51.9	26.36	21.1
		5*A10+A3*B3+B30*A30+A36*B36+A11					[220]
$C_8H_8O_3$		4-hydroxyphenylacetic acid					
	423.6	28.4	0	67.04	56.1	28.4	23.9
		4*A10+A11+A12+A2+A36*B36+A31					[215]
$C_8H_8O_3$		4-methoxybenzoic acid					
	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
		4*A10+2*A12+A1+A36*B36+A32					[215,394]
$C_8H_9ClO_3$		(4-chloro-2-methylphenoxy)acetic acid					
	392.9	29.98	0	76.31	73.3	29.98	28.8
		3*A10+2*A12+A11+A22*C22+A36*C36+A32+A2+A1					[221]
C_8H_9NO		4-aminoacetophenone					
	379.2	38	0	100.2	58.2	38	22.1
		4*A10+2*A12+A35+A45+A1					[280]
C_8H_9NO		3-aminoacetophenone					
	371.2	29	0	78.12	58.2	29	21.6
		4*A10+2*A12+A35+A45+A1					[280]
C_8H_9NO		acetanilide					
	387.5	21.65	0	55.87	48.6	21.6	18.8
		5*A10+A12+A1+A60					[216]
$C_8H_9NO_2$		methyl 4-aminobenzoate					
	385.1	22.55	0	58.56	61.3	22.55	23.6
		4*A10+2*A12+A1+A45+A38					[239]
$C_8H_9NO_2$		*o*-hydroxyacetanilide					
	364.5	21.25	0	58.3	54.0	21.25	23.8
		4*A10+A60+A1+2*A12+A31					[216]
$C_8H_9NO_2$		*p*-hydroxyacetanilide					
	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
		4*A10+A60+A1+2*A12+A31					[239,394]
$C_8H_9NO_2$		methyl N-phenylcarbamate					
	325	14.56	0	44.77	57.8	14.56	18.8
		5*A10+A12+A1+A69					[216]
$C_8H_9ClNO_5PS$		O-(2-chloro-4-nitrophenyl)O,O-dimethyl phosphorothioate					
	323.9	29.08	0	89.78	70.0	29.08	22.7
		2*A1+3*A10+3*A12+A22*C22+A50+A79					[221]
$C_8H_9O_3PS$		2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulfide					
	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)
		*A*14+3**A*15+*A*19+*A*19+4**A*10+*A*130+*A*1					[221]
C_8H_{10}		*o*-xylene					
	247.8	13.6	0	54.9	45.6	13.6	11.3
		2**A*1+4**A*10+2**A*11					[216]
C_8H_{10}		*m*-xylene					
	225.3	11.57	0	51.4	45.6	11.57	10.3
		2**A*1+4**A*10+2**A*11					[216]
C_8H_{10}		*p*-xylene					
	286.3	17.11	0	59.77	45.6	17.11	13.1
		2**A*1+4**A*10+2**A*11					[216]
C_8H_{10}		ethylbenzene					
	178.2	9.16	0	51.43	52.2	9.16	9.3
		*A*1+*A*2+5**A*10+*A*11					[216]
$C_8H_{10}N_4O_2$		caffeine					
	426	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
		2**A*14+3**A*15+2**A*125+3**A*1+2**A*19+*A*18**B*18+*A*119+*A*118					[227,395]
$C_8H_{10}NO_5PS$		O,O-dimethyl O-4-nitrophenyl phosphorothioate					
	308.2	20.07	0	65.12	68.7	20.07	21.2
		4**A*10+2**A*12+2**A*1+*A*50+*A*79					[215]
$C_8H_{10}O$		2,3-dimethylphenol					
	346	21.02	0	60.75	51.0	21.02	17.6
		3**A*10+2**A*11+*A*12+2**A*1+*A*31					[215]
$C_8H_{10}O$		2,5-dimethylphenol					
	348	23.38	0	67.18	51.0	23.38	17.7
		3**A*10+2**A*11+*A*12+2**A*1+*A*31					[215]
$C_8H_{10}O$		2,6-dimethylphenol					
	318.9	18.9	0	59.27	51.0	18.9	16.3
		3**A*10+2**A*11+*A*12+2**A*1+*A*31					[215]
$C_8H_{10}O$		3,4-dimethylphenol					
	334	18.13	0	54.28	51.0	18.13	17.0
		3**A*10+2**A*11+*A*12+2**A*1+*A*31					[215]
$C_8H_{10}O$		3,5-dimethylphenol					
	336.8	18	0	53.44	51.0	18.0	17.2
		3**A*10+2**A*11+*A*12+2**A*1+*A*31					[215]
$C_8H_{10}O_2S$		benzylmethylsulfone					
	400.5	25.52	0	63.73	52.5	25.52	21.0
		5**A*10+*A*11+*A*1+*A*2+*A*88					[276]
$C_8H_{11}N$		2,5-dimethylaniline					
	279	13.7	0	49.1	52.1	13.7	14.5
		3**A*10+2**A*11+*A*12+2**A*1+*A*45					[51]
$C_8H_{11}N$		N,N-dimethylaniline					
	275.6	11.56	0	46.28	42.5	11.56	11.7
		5**A*10+*A*12+*A*43+2**A*1					[51]
$C_8H_{11}N$		exo-2-cyanobicyclo[2.2.1]heptane					
	237.7	7.93	33.4				
	298.8	2.94	9.83	43.2	44.0	10.87	13.1
		2**A*14+*A*15+2**A*16+*A*16+*A*56					[216]
$C_8H_{11}N$		endo-2-cyanobicyclo[2.2.1]heptane					
	177.3	2.25	12.7				
	331.2	2.96	8.94	21.6	44.0	7.18	14.6
		2**A*14+*A*15+2**A*16+*A*56+*A*16					[216]
$C_8H_{11}N$		2,4,6-trimethylpyridine					
	229.0	9.54	0	41.64	50.0	9.54	11.4
		3**A*1+3**A*11+2**A*10+*A*41					[216]
$C_8H_{11}N_5$		6,8,9-trimethyladenine					
	438	23.1	0	52.74	54.4	23.1	23.8
		*A*14+2**A*15+3**A*19+3**A*1+*A*118+*A*119+2**A*41+*A*10+*A*12+*A*44					[240]
$C_8H_{11}N_5O_2$		2-amino-9-[(2-hydroxyethoxy)methyl]-9H-purine					
	462.2	42.2	0	91.3	86.5	42.2	40.0
		*A*14+2**A*15+2**A*19+*A*18**B*18+2**A*41+*A*45+*A*118+*A*119+3**A*2+*A*30**F*30+*A*32					[203]
$C_8H_{11}N_5O_3$		2-amino-9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one					
	528.2	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)	
		2*A14+3*A15+3*A19+A18*B18+A124+2*A118+A45+A119+3*A2+A32+A30*F30						[203]
C_8H_{12}		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	
		2*A14+2*A15+2*A16+2*A18						[100]
C_8H_{12}		cycloocta-1,5-diene						
	194.4	−0.38						
	204	9.83	0	48.2	45.4	9.83	9.3	
		A14+5*A15+4*A18						[216]
$C_8H_{12}NO_5PS_2$		O,O-dimethyl O-(4-aminosulfonylphenyl)phosphorodithioate						
	344.2	26.21	0	76.13	79.4	26.21	27.3	
		2*A1+4*A10+2*A12+A96+A79						[221]
$C_8H_{12}N_2$		tetramethylsuccinonitrile						
	345	18.1	52.48					
	442	7.15	16.17	68.64	60.1	25.25	26.6	
		4*A1+2*A4*B4+2*A56						[216]
$C_8H_{12}N_2O_2$		1,6-hexamethylene diisocyanate						
	206.1	18.64	0	90.46	102.2	18.64	21.1	
		6*A2*B2+2*A58						[216]
$C_8H_{12}N_2O_3$		barbitol						
	462.6	24.98	0	54	63.1	24.98	29.2	
		A14+3*A15+A128+A124+2*A1+2*A2+A17						[241]
$C_8H_{12}N_4O_{10}$		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	
		2*A4*B4+3*A2+2*A1+4*A50+A38						[122]
$C_8H_{12}N_4O_{10}$		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	
		2*A1+2*A4*B4+3*A2+4*A50+A38						[122]
$C_8H_{12}O_2$		1,4-cyclooctanedione						
	341.2	11.92	0	34.95	49.2	11.92	16.8	
		A14+5*A15+2*A114						[114]
$C_8H_{13}ClN_2O_2$		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	
		A14+3*A15+2*A19+A124+A125+4*A1+A4*B4+A22*C22						[221]
C_8H_{14}		*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	
		2*A14+A15+A1+3*A16						[216]
C_8H_{14}		*exo*-2-methylbicyclo[2.2.1]heptane						
	164.1	8.38	0	51.0	43.8	8.38	7.2	
		2*A14+A15+A1+3*A16						[216]
C_8H_{14}		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	
		2*A14+2*A16+2*A15						[215]
C_8H_{14}		cyclooctene						
	190.1	9.8	51.55					
	259.2	1.81	6.98	58.53	48.7	11.61	12.6	
		A14+5*A15+2*A18						[161]
$C_8H_{14}N_4OS$		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	
		A14+3*A15+2*A19+4*A1+A4+A125+A84+A45+2*A118						[215]
$C_8H_{14}N_5Cl$		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	
		3*A41+3*A12+2*A44+A22*F22+3*A1+A2+A3*B3						[221]
$C_8H_{14}N_6O_{10}$		1,7-diacetoxy-2,4,6-trinitro-2,4,6-triazaheptane						
	422.5	38.49	0	91.11	214.5	38.49	90.6	
		2*A1+4*A2+2*A38+3*A51+3*A47						[216]
$C_8H_{14}O$		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	
		2*A14+3*A15+2*A16+A112						[216]
$C_8H_{14}O_4$		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}		*trans*-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}		*cis*-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}		*trans*-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}		*cis*-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}		*trans*-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}		*cis*-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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		2*A1+5*A2*B2+A35					[216]
$C_8H_{16}O_2$		octanoic acid					
	289.7	21.35	0	73.8	86.9	21.35	25.2
		6*A2*B2+A1+A36					[216]
$C_8H_{16}O_2$		2,2,6,6-tetramethyl-1,3-dioxane					
	250.6	10.9	0	43.5	48.1	10.9	12.1
		A14+3*A15+2*A112+4*A1+2*A17					[47]
$C_8H_{16}O_2$		butyl butanoate					
	181.68	14.93	0	82.18	78.5	14.93	14.3
		2*A1+5*A2+A38					[216]
$C_8H_{16}O_2$		hexyl ethanoate					
	212.1	19.83	0	93.49	89.5	19.83	19.0
		2*A1+5*A2*B2+A38					[216]
C_8H_{18}		*n*-octane					
	216.38	20.74	0	95.86	91.1	20.74	19.7
		2*A1+6*A2*B2					[216]
C_8H_{18}		2,2,4-trimethylpentane					
	165.3	9.04	0	54.7	43.8	9.04	7.3
		5*A1+A4+A2+A3					[216]
C_8H_{18}		2,2,4-trimethylpentane					
	165.8	9.2	0	55.52	43.8	9.2	7.3
		5*A1+A2+A4+A3					[216]
C_8H_{18}		2,3,4-trimethylpentane					
	163.6	9.27	0	56.65	38.8	9.27	6.4
		5*A1+3*A3					[216]
C_8H_{18}		3-methylheptane					
	152.6	11.7	0	76.6	64.9	11.7	9.9
		3*A1+4*A2+A3					[216]
C_8H_{18}		2-methylheptane					
	164.2	11.92	0	72.62	64.9	11.92	10.7
		3*A1+4*A2+A3					[216]
C_8H_{18}		2,2,3,3-tetramethylbutane					
	152.5	2	13.11				
	373.9	7.54	20.16	33.28	35.8	9.54	13.4
		6*A1+2*A4					[216]
C_8H_{18}		4-methylheptane					
	152.2	10.84	0	71.22	64.9	10.84	9.9
		3*A1+A3+4*A2					[215]
$C_8H_{18}Cl_2Sn$		di-*n*-butyltindichloride					
	316.2	22.75	0	71.95	86.1	22.75	27.2
		2*A1+6*A2+2*A2*D22+A110					[130]
$C_8H_{18}N_2$		1,1-dimethylazoethane					
	242.6	4.89	20.16				
	258.6	10.28	39.75	59.91	56.3	15.17	14.6
		6*A1+2*A4*B4+2*A42					[42]
$C_8H_{18}N_2O$		1,1-dimethylazoxyethane					
	268	8.34	31.12				
	288.4	11.52	39.94	71.06	64.9	19.86	18.7
		6*A1+2*A4*B4+A54+A42					[42]
$C_8H_{18}N_2O_2$		*bis*-hydroxyethylpiperazine					
	405	25.9	0	63.95	80.2	25.9	32.5
		A14+3*A15+2*A119+4*A2+2*A30*D30					[216]
$C_8H_{18}N_4O_4$		N,N′-dimethyl-N,N′-dinitro-1,6-hexanediamine					
	331	61.68	0	186.35	113.0	61.68	37.4
		6*A2+2*A1+2*A43+2*A51					[225]
$C_8H_{18}O_2$		1,8-octanediol					
	332.8	36.1	0	108.47	111.0	36.1	36.9
		8*A2*B2+2*A30*B30					[215]
$C_8H_{18}O_4$		2,5,8,11-tetraoxadodecane					
	229.3	23.71	0	103.34	96.8	23.71	22.2
		2*A1+6*A2+4*A32					[216]
$C_8H_{18}S$		di-*n*-butyl sulfide					
	198.1	19.41	0	93.85	80.1	19.41	15.9
		2*A1+6*A2+A84					[216]
$C_8H_{18}S$		1-octanethiol					
	224	24.27	0	108.35	105.9	4.27	23.7
		A1+7*A2*B2+A86					[216]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_8H_{19}NSi$		N-(β-trimethylsilylethyl)trimethylenimine					
	199.4	12.9	0	64.68	57.7	12.9	11.5
		*A*14+*A*15+*A*119+3**A*1+2**A*2+*A*109					[216]
$C_8H_{20}Ge$		tetraethylgermane					
	180.3	12.31	0	68.29	63.7	12.31	11.5
		4**A*1+4**A*2+*A*102					[216]
$C_8H_{20}O_4Si$		tetraethoxysilane					
	187.7	13.2	70.32				
	191.0	11.14	58.33	128.66	90.6	24.34	17.3
		4**A*1+4**A*2+4**A*32+*A*109					[10]
$C_8H_{20}Pb$		tetraethyllead					
	141.4	9.11	0	64.43	68.7	9.11	9.7
		4**A*1+4**A*2+*A*106					[216]
$C_8H_{20}Si$		tetraethylsilane					
	189.4	13.01	0	68.72	71.8	13.01	13.6
		4**A*1+4**A*2+*A*109					[227]
$C_8H_{20}Sn$		tetraethyltin					
	142.1	9.15	0	64.35	74.6	9.15	10.6
		4**A*1+4**A*2+*A*110					[216]
$C_8H_{24}O_4Si_4$		octamethylcyclotetrasiloxane					
	258	4.87	18.86				
	290.5	23.77	81.81	100.67	58.6	28.63	17.0
		8**A*1+*A*14+5**A*15+4**A*139+4**A*112					[216,98,121]
$C_8H_{28}N_4Si_4$		octamethylcyclotetrasilazane					
	367.7	25.05	0	68.13	62.5	25.05	23.0
		8**A*1+*A*14+5**A*15+4**A*139+4**A*121					[216]
$C_9H_4Cl_3NO_2S$		2-[(trichloromethyl)thiol]-1H-isoindole-1,3(2H)-dione					
	454.2	35.49	0	78.14	74.8	35.49	34.0
		*A*14+2**A*15+*A*128+2**A*19+4**A*10+*A*4**B*4+*A*84+3**A*22**E*22					[215]
$C_9H_4Cl_4O_4$		methyl tetrachloroterephthalic acid ester					
	444.3	16.89	0	38.01	75.1	16.89	33.4
		4**A*2**F*22+*A*38+*A*36**F*36+6**A*12+*A*1					[221]
$C_9H_4Cl_8O$		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**A*14+*A*15+3**A*17+2**A*19+4**A*16+*A*112+8**A*22**G*22					[232]
$C_9H_4O_5$		trimellitic anhydride 1,2,4-benzenetricarbozylic acid					
	385	10.46	0	27.18	33.3	10.46	12.8
		*A*14+2**A*15+3**A*10+*A*12+*A*117+2**A*19					[216]
$C_9H_5N_4Cl_3$		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**A*10+5**A*12+3**A*22**G*22+3**A*41+*A*44					[221]
$C_9H_6Cl_2N_2O_3$		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
		*A*14+2**A*15+*A*125+2**A*22**E*22+3**A*10+3**A*12+*A*1+*A*126					[221]
$C_9H_6Cl_6O_4S$		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**A*14+3**A*15+6**A*22**D*22+3**A*17+2**A*19+*A*136+2**A*16					[221]
$C_9H_6O_2$		coumarin					
	342.1	19.14	0	55.95	48.0	19.14	16.4
		*A*14+3**A*15+*A*115+*A*18+*A*18+*A*19+*A*19+4**A*10					[82]
$C_9H_6O_2$		chromone					
	330.3	17.31	0	52.41	43.3	17.31	14.3
		*A*14+3**A*15+4**A*10+*A*114+*A*112+2**A*18**B*18+2**A*19					[215,216]
$C_9H_7Cl_3O_3$		2-(2,4,5-trichlorophenoxy)propanoic acid					
	450.6	39.58	0	87.83	76.0	39.58	34.2
		2**A*10+4**A*12+3**A*22**E*22+*A*36**E*36+*A*32+*A*3**B*3+*A*1					[221]
$C_9H_7Cl_3O_3$		methyl 2-(2,4,5-trichlorophenoxy)acetate					
	361.9	30.46	0	84.18	70.5	30.46	25.5
		2**A*10+4**A*12+*A*2+*A*32+*A*38+3**A*22**E*22+*A*1					[221]
C_9H_7N		quinoline					
	220	0.07	0.31				
	258.4	10.66	41.27	41.58	47.9	10.73	12.4
		7**A*10+2**A*12+*A*41					[216]
C_9H_7N		isoquinoline					
	299.6	13.54	0	45.21	47.9	13.54	14.3
		7**A*10+2**A*12+*A*41					[216]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_9H_7N_3S$		5-methyl-1,2,4-triazolo[3,4-*b*]benzothiazole					
	460.2	24.07	0	52.3	49.1	24.07	22.6
		2*A14+2*A15+A1+3*A10+3*A19+A11+A119+2*A118+A131+A18*B18					[221]
C_9H_8		indene					
	271.7	10.2	0	37.54	42.7	10.2	11.6
		4*A10+2*A15+A14+2*A18+2*A19					[216]
$C_9H_8Cl_2O_3$		methyl 3,6-dichloro-2-methoxybenzoate					
	304.6	18.49	0	60.7	64.8	18.49	19.7
		4*A12+2*A10+2*A1+A38*D38+2*A22*D22+A32					[215]
$C_9H_8Cl_2O_3$		2-(2,4-dichlorophenoxy)propanoic acid					
	389.2	30.43	0	78.18	74.8	30.43	29.1
		3*A10+3*A12+2*A22*D22+A36*D36+A32+A1+A3*B3					[215]
$C_9H_8Cl_2O_3$		methyl 2,4-dichlorophenoxyacetate					
	315.4	25.1	0	79.59	69.3	25.1	21.8
		2*A22*D22+A1+3*A12+3*A10+A38+A32+A2					[232]
$C_9H_8O_2$		cinnamic acid					
	406.2	22.63	0	55.71	52.1	22.63	21.2
		5*A10+A12+A6+A36+A6*B6					[215]
$C_9H_8O_2$		allocinnamic acid					
	341.2	16.95	0	49.68	52.1	16.95	17.8
		5*A10+A12+A6+A36+A6*B6					[215]
$C_9H_9BrO_3$		(*dl*) 2-(*p*-bromophenoxy)propanoic acid					
	385	31.8	0	82.59	74.9	31.8	28.8
		4*A10+2*A12+A1+A3*B3+A36*C36+A21+A32					[220]
$C_9H_9BrO_3$		(*d*) 2-(*p*-bromophenoxy)propanoic acid					
	380	27.61	0	72.67	74.9	27.61	28.5
		4*A10+2*A12+A1+A3*B3+A36*C36+A21+A32					[220]
$C_9H_9BrO_3$		(*dl*) 3-(*m*-bromophenyl)-3-hydroxypropanoic acid					
	349	26.78	0	76.73	74.6	26.78	26.1
		4*A10+A12+A11+C30*A30+A36*C36+A21+A2+A3*B3					[220]
$C_9H_9BrO_3$		(*d*) 3-(*m*-bromophenyl)-3-hydroxypropanoic acid					
	350	23.85	0	68.14	74.6	23.9	26.1
		4*A10+A12+A11+C30*A30+A36*C36+A21+A3*B3+A2					[220]
$C_9H_9BrO_3$		(*dl*) 3-(*p*-bromophenyl)-3-hydroxypropanoic acid					
	371	28.87	0	77.82	74.6	28.9	27.7
		4*A10+A12+A11+A21+C30*A30+A36*C36+A3*B3+A2					[220]
$C_9H_9BrO_3$		(*d*) 3-(*p*-bromophenyl)-3-hydroxypropanoic acid					
	398	35.56	0	89.36	74.6	35.56	29.7
		4*A10+A12+A11+A21+C30*A30+A36*C36+A3*B3+A2					[220]
$C_9H_9ClO_3$		(*dl*) 2-(*o*-chlorophenoxy)propanoic acid					
	388	32.22	0	83.03	73.4	32.22	28.5
		4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32					[220]
$C_9H_9ClO_3$		(*d*) 2-(*o*-chlorophenoxy)propanoic acid					
	369	26.78	0	72.57	73.4	26.78	27.1
		4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32					[220]
$C_9H_9ClO_3$		(*dl*) 2-(*m*-chlorophenoxy)propanoic acid					
	386	33.05	0	85.63	73.4	33.05	28.3
		4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32					[220]
$C_9H_9ClO_3$		(*d*) 2-(*m*-chlorophenoxy)propanoic acid					
	367.5	29.71	0	80.83	73.4	29.71	27.0
		4*A10+2*A12+A1+A3*B3+A36*C36+A22*C22+A32					[220]
$C_9H_9ClO_3$		(*dl*) 3-(*p*-chlorophenyl)-3-hydroxypropanoic acid					
	357	29.71	0	83.21	73.1	29.71	26.1
		4*A10+A12+A22*C22+C30*A30+A36*C36+A2+A3*B3+A11					[220]
$C_9H_9ClO_3$		(*d*) 3-(*p*-chlorophenyl)-3-hydroxypropanoic acid					
	385	28.03	0	72.81	73.1	28.03	28.1
		4*A10+A12+A11+A22*C22+C30*A30+A36*C36+A3*B3+A2					[220]
$C_9H_9ClO_3$		(*dl*) 3-(*m*-chlorophenyl)-3-hydroxypropanoic acid					
	340	23.85	0	70.14	73.1	23.85	24.9
		4*A10+A12+A11+A22*C22+C30*A30+A36*C36+A2+A3*B3					[220]
$C_9H_9ClO_3$		(*d*) 3-(*m*-chlorophenyl)-3-hydroxypropanoic acid					
	368	28.03	0	76.18	73.1	28.03	26.9
		4*A10+A12+A11+A22*C22+C30*A30+A36*C36+A3*B3+A2					[220]
$C_9H_9ClO_3$		(4-chloro-*o*-tolyloxy)acetic acid					
	392.9	29.98	0	76.3	73.3	29.98	28.8
		3*A10+2*A12+A11+A2+A1+A22*C22+A32+A36*C36					[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)
$C_9H_9Cl_2NO$		3′,4′-dichloropropionanilide					
	363.7	18.26	0	50.22	58.3	18.26	21.2
		$A1+A2+A60+3*A12+3*A10+2*A22*C22$					[215]
$C_9H_9FO_3$		(*dl*) 3-(*m*-fluorophenyl)-3-hydroxypropanoic acid					
	290	20.5	0	70.7	73.5	20.5	21.3
		$4*A10+A12+A11+A24+C30*A30+A36*C36+A2+A3*B3$					[220]
$C_9H_9FO_3$		(*d*) 3-(*m*-fluorophenyl)-3-hydroxypropanoic acid					
	311	24.27	0	78.03	73.5	24.27	22.9
		$4*A10+A12+A11+A24+C30*A30+A36*C36+A3*B3+A2$					[220]
$C_9H_9FO_3$		(*d*) 3-(*o*-fluorophenyl)-3-hydroxypropanoic acid					
	342	27.2	0	79.52	73.5	27.2	25.2
		$4*A10+A11+A12+A24+C30*A30+A36*C36+A2+A3*B3$					[220]
$C_9H_9FO_3$		(*d*) 3-(*o*-fluorophenyl)-3-hydroxypropanoic acid					
	348	22.59	0	64.92	73.5	22.59	25.6
		$4*A10+A11+A12+A24+C30*A30+A36*C36+A3*B3+A2$					[220]
$C_9H_9FO_3$		(*dl*) 3-(*p*-fluorophenyl)-3-hydroxypropanoic acid					
	362	27.61	0	76.28	73.5	27.61	26.6
		$4*A10+A11+A12+A24+C30*A30+A36*C36+A2+A3*B3$					[220]
$C_9H_9FO_3$		(*d*) 3-(*p*-fluorophenyl)-3-hydroxypropanoic acid					
	381	30.96	0	81.26	73.5	30.96	28.0
		$4*A10+A11+A12+A24+C30*A30+A36*C36+A3*B3+A2$					[220]
$C_9H_9NO_4$		[(benzoylamino)oxy] acetic acid					
	416.9	31.46	0	75.46	72.9	31.46	30.4
		$5*A10+A12+A60+A32+A2+A36*C36$					[215]
$C_9H_9NO_5$		(*dl*) 2-(*p*-nitrophenoxy)propanoic acid					
	411.4	32.22	0	78.31	74.9	32.22	30.8
		$4*A10+2*A12+A1+A3*B3+A36*C36+A32+A50$					[220]
$C_9H_9NO_5$		(*d*) 2-(*p*-nitrophenoxy)propanoic acid					
	362	20.92	0	57.79	74.9	20.92	27.1
		$4*A10+2*A12+A1+A3*B3+A36*C36+A32+A50$					[220]
C_9H_{10}		indane					
	221.8	8.6	0	38.77	45.9	8.6	10.2
		$4*A10+2*A19+A14+2*A15$					[216]
C_9H_{10}		α-methylstyrene					
	250.8	11.92	0	47.55	53.8	11.92	13.5
		$5*A10+A12+A1+A5+A7$					[216]
$C_9H_{10}Cl_2N_2O$		3-(3,4-dichlorophenyl)-1,1-dimethylurea					
	429.7	33.89	0	78.87	64.8	33.89	27.84
		$2*A1+2*A22*C22+3*A12+3*A10+A64*B64$					[232]
$C_9H_{10}BrClN_2O_2$		3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea					
	369.8	26.54	0	71.79	68.7	26.54	25.4
		$2*A1+3*A10+3*A12+A32+A22*D22+A21+A64$					[221]
$C_9H_{10}Cl_2N_2O_2$		N'-(3,4-dichlorophenyl)-N-methoxy-N-methylurea					
	365.8	26.56	0	72.61	67.3	26.56	24.6
		$2*A22*D22+A32+A64+2*A1+3*A12+3*A10$					[215]
$C_9H_{10}O$		chroman					
	269.8	16.26	0	60.24	50.8	16.26	13.7
		$A14+3*A15+A19+A19+A112+4*A10$					[216]
$C_9H_{10}O$		isochroman					
	277.5	16.75	0	60.35	50.8	16.75	14.1
		$A14+3*A15+2*A19+A112+4*A10$					[216]
$C_9H_{10}O$		cinnamyl alcohol					
	308.2	15.73	0	51.04	49.0	15.73	15.1
		$5*A10+A12+2*A6+A2+A30$					[220]
$C_9H_{10}O$		4-ethylbenzoic acid					
	386.2	14.06	0	36.4	50.7	14.06	19.6
		$4*A10+A11+A12+A1+A2+A36$					[220]
$C_9H_{10}O_2$		hydrocinnamic acid					
	321.2	17.68	0	55.04	55.1	17.68	17.7
		$5*A10+A11+2*A2+A36$					[215]
$C_9H_{10}O_2$		phenyl glycidyl ether					
	279.8	17.32	0	61.9	61.3	17.32	17.2
		$A14+A112+A32*B32+16+A2+5*A10+A12$					[135]
$C_9H_{10}O_2S$		tolyl vinyl sulfone					
	340.4	10.88	0	31.96	53.0	10.88	18.0
		$4*A10+A11+A1+A5+A6+A88+A12$					[238]

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)
$C_9H_{10}O_3$	(*dl*) 3-phenyl-3-hydroxypropanoic acid					
366	29.71	0	81.17	59.2	29.71	21.7
	5*A10+A11+A2+A3*B3+B30*A30+A36*B36					[220]
$C_9H_{10}O_3$	(*d*) 3-phenyl-3-hydroxypropanoic acid					
391	32.64	0	83.47	59.2	32.64	23.1
	5*A10+A11+A2+A3*B3+A30*B30*+B36*A36					[220]
$C_9H_{10}O_3$	(*dl*) 2-phenoxypropionic acid					
388	33.05	0	85.19	58.2	33.05	22.6
	5*A10+A12+A1+A3*B3+A36*B36+A32*B32					[220]
$C_9H_{10}O_3$	(*d*) 2-phenoxypropionic acid					
359	22.59	0	62.93	58.2	22.59	20.9
	5*A10+A12+A1+A3*B3+A36*B36+A32*B32					[220]
$C_9H_{10}O_3$	4-methoxyphenylacetic acid					
358.1	21.8	0	60.88	58.1	21.8	20.8
	4*A10+A11+A12+A1+A2+A36*B36+A32*B32					[215]
$C_9H_{10}O_3$	4-hydroxyphenylpropionic acid					
402.5	28.9	0	71.8	63.2	28.9	25.5
	4*A10+A11+A12+2*A2+A36*B36+A31					[215]
$C_9H_{10}O_3$	4-ethoxybenzoic acid					
472.8	29.4	0	62.18	60.2	29.4	28.5
	4*A10+2*A12+A1+A2+A36*B36+A32*B32					[215]
$C_9H_{10}O_4$	(*dl*) erythro phenylglyceric acid					
395	31.38	0	79.44	71.9	31.38	28.4
	5*A10+A11+2*A3*B3+2*C30*A30+A36*C36					[220]
$C_9H_{10}O_4$	(*d*) erythro phenylglyceric acid					
371.5	23.43	0	63.07	71.9	23.43	26.7
	5*A10+A11+2*A3*B3+2*C30*A30+A36*C36					[220]
$C_9H_{11}BrN_2O$	N′-(4-bromophenyl)-N-methoxy-N-methyl urea					
368.3	24.44	0	66.36	67.4	24.44	24.8
	2*A1+A32*C32+4*A10+2*A12+A64*C64*+A21					[215]
$C_9H_{11}ClN_2O_2$	N′-(4-chlorophenyl)-N-methoxy-N-methyl urea					
353.4	22.54	0	63.78	66.0	22.54	23.3
	2*A1+4*A10+2*A12+A22*C22+A64*C64+A32					[215]
$C_9H_{11}ClN_2O$	3-(4-chlorophenyl)-1,1-dimethyl urea					
447.6	29.46	0	65.82	66.0	29.46	29.6
	2*A1+A64*B64+A22*B22+2*A12+4*A10					[215]
$C_9H_{11}ClO_3$	2-(4-chloro-2-methylphenoxy)propanoic acid					
366.2	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]
$C_9H_{11}Cl_3NO_3PS$	O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate					
315	24.53	0	77.86	87.5	24.53	27.6
	4*A12+A10+A41+3*A22*E22+2*A1+2*A2+A79					[215]
$C_9H_{11}N$	1,2,3,4-tetrahydroquinoline					
290	11.81	0	40.73	51.8	11.81	15.0
	A14+3*A15+A121+A19+4*A10+A19					[215]
$C_9H_{11}N$	5,6,7,8-tetrahydroquinoline					
222.7	9.08	0	40.75	53.1	9.08	11.8
	A14+3*A15+3*A10+A41+A19+A19					[215]
$C_9H_{11}NO_2$	ethyl phenyl carbamate					
326	16.27	0	49.79	64.9	16.27	21.2
	5*A10+A12+A1+A2+A69					[102]
$C_9H_{11}NO_2$	ethyl 4-aminobenzoate					
362.8	23.56	0	64.94	68.5	23.56	24.8
363.2	22.0	0	60.6	68.5	22.0	24.8
	4*A10+2*A12+A1+A2+A38+A5					[215,395]
$C_9H_{11}NO_2$	*p*-methoxyacetanilide					
400.3	27.82	0	69.51	56.0	27.82	22.4
	2*A1+4*A10+2*A12+A32+A60					[239]
C_9H_{12}	1,2,3-trimethylbenzene					
218.7	0.66	3				
230.3	1.33	5.8				
247.8	8.18	33.01	41.81	46.2	10.17	11.4
	3*A1+3*A10+3*A11					[216]
C_9H_{12}	1,2,4-trimethylbenzene					
229.3	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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
C_9H_{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}		*n*-propylbenzene					
	173.6	9.27	0	53.39	59.3	9.27	10.3
		5*A10+A1+2*A2+A11					[215]
$C_9H_{12}ClN_5$		6-chloro-N-cyclopropyl-N′-(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]
$C_9H_{12}N_2O$		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]
$C_9H_{12}N_4O_2$		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]
$C_9H_{13}BrN_2O_2$		5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-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]
$C_9H_{13}ClN_6$		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]
$C_9H_{13}N_5$		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]
$C_9H_{14}ClN_5$		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]
$C_9H_{14}O_6$		glyceryl triacetate					
	275.3	25.8	0	93.73	80.2	25.8	22.1
		2*A2+3*A1+A3*B3+3*A38					[216]
$C_9H_{15}N_3O_8$		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}		*trans*-hexahydroindane					
	213.9	10.9	0	50.98	48.4	10.9	10.4
		2*A14+3*A15+2*A16					[184]
C_9H_{16}		*cis*-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]
$C_9H_{16}ClN_5$		6-chloro-N-(1,1-dimethylethyl)-N′-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]
$C_9H_{16}N_4OS$		N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N′-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]
$C_9H_{16}O_4$		azelaic acid					
	380	32.67	0	85.97	97.5	32.67	37.1
		2*A36*B36+7*A2*B2					[215]
$C_9H_{17}N$		*trans*-(R,S)-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}		*n*-butylcyclopentane					
	165.2	11.31	0	68.49	65.0	11.31	10.7
		A14+A16+3*A2+2*A15					[216]
C_9H_{18}		*n*-propylcyclohexane					
	178.3	10.37	0	58.19	61.6	10.37	11.0
		A14+A1+A16+2*A2+3*A15					[215]
$C_9H_{18}N_2O_2S$		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)
		5*A1+A4+A2+A7+A42+A84+A69					[215]
$C_9H_{18}N_6$		1,3,5-tris(dimethylamino)-*s*-triazine					
	444.4	23.01	0	51.78	49.0	23.01	21.8
		3*A41+3*A12+3*A43+6*A1					[215]
$C_9H_{18}N_6$		1-(ethylamino)-3,5-bis(dimethylamino)-*s*-triazine					
	333	16.74	0	50.27	55.5	16.74	18.5
		3*A41+3*A12+2*A43+A44+5*A1+A2					[215]
$C_9H_{18}O$		nonanal					
	253.9	29.6	0	116.6	104.4	29.6	26.5
		A1+7*A2*B2+A34					[43]
$C_9H_{18}O$		5-nonanone					
	269.3	24.94	92.59				
	451.8	11.27	24.94	117.5	82.5	36.2	37.3
		2*A1+6*A2+A35					[215]
$C_9H_{18}O_2$		nonanoic acid					
	268	5.61	20.92				
	285.5	20.31	71.13	92.05	96.3	25.91	27.5
		7*A2*B2+A1+A36					[215]
C_9H_{20}		nonane					
	217.2	6.28	28.91				
	219.7	15.48	70.29	99.2	100.5	21.76	22.1
		2*A1+7*A2*B2					[215, 216]
C_9H_{20}		2,2,3,3-tetramethylpentane					
	174.5	7.33	42.0				
	263.4	2.33	8.9	50.9	42.9	9.66	11.3
		6*A1+A2+2*A4					[216]
C_9H_{20}		2,2,4,4-tetramethylpentane					
	206.7	9.75	0	47.17	42.9	9.75	8.9
		6*A1+A2+2*A4					[216]
C_9H_{20}		3,3-diethylpentane					
	208.3	0.48	2.32				
	210.4	0.81	3.85				
	240.1	10.09	42.02	48.2	64.0	11.38	15.4
		4*A1+4*A2+A4					[216]
$C_9H_{20}N_2O$		1,3-dibutylurea					
	311.5	11.1	35.63				
	346.9	14.87	42.87	78.5	79.4	25.97	27.6
		2*A1+A66+6*A2					[216]
$C_9H_{20}N_2O$		1,1,3,3-tetraethylurea					
	253	20.55	0	81.23	79.5	20.55	20.1
		4*A1+4*A2+A63					[169, 124]
$C_9H_{20}O$		2,2,4,4-tetramethylpentan-3-ol					
	263	1.9	7.22				
	322	7.3	22.67	29.9	21.2	9.2	6.8
		6*A1+2*A4+A3*B3+A30					[216]
$C_9H_{20}O_2$		1,9-nonanediol					
	319.6	36.4	0	113.89	120.2	36.4	38.4
		9*A2*B2+2*A30*B30					[215]
$C_9H_{20}O_2S$		3(*n*-hexylthio)-1,2-propanediol					
	290.8	48.5	0	166.78	109.3	48.5	31.8
		A1+5*A2*B2+A84+2*A30*C30+A3*B3+2*A2*B2					[217]
$C_9H_{20}O_3$		3(*n*-hexyloxy)-1,2-propanediol					
	272.9	10.2	0	37.38	111.9	10.2	30.6
		A1+5*A2*B2+A32+2*A30*C30+A3*B3+2*A2					[243]
$C_9H_{20}S$		1-nonanethiol					
	267.7	33.5	0	125.14	115.2	33.5	30.9
		A1+8*A2*B2+A86					[136]
$C_9H_{24}Si_2$		1,3-hexamethyldisilylpropane					
	223.7	16.05	0	71.75	72.7	16.05	16.3
		6*A1+2*A109+3*A2					[216]
$C_9H_{24}Si_3$		1,1,3,3,5,5-hexamethyl-1,3,5-trisilacyclocyclohexane					
	269.3	16.5	0	61.26	45.9	16.5	12.4
		A14+3*A15+3*A139+6*A1					[216]
$C_{10}F_{14}$		perfluorobicyclo[4.4.0]deca-1,6-diene					
	200	0.75	3.77				
	233	1.11	4.77				
	264	10.47	39.66	49.2	73.7	12.34	12.9
		2*A14+4*A15+6*A17+12*A28+2*A19+2*A23+2*A19					[216]
$C_{10}F_{18}$		*cis*-perfluorodecalin					

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)
	232.5	4.24	18.2				
	266.7	10.3	38.62	56.82	50.3	14.54	13.4
		2*A14+4*A15+10*A17+18*A28					[216]
$C_{10}F_{18}$		*trans*-perfluorodecalin					
	294.6	17.96	0	60.96	50.3	17.96	14.8
		2*A14+4*A15+10*A17+18*A28					[216]
$C_{10}H_2O_6$		pyromellitic dianhydride 1,2,5,6-benzenetetracarboxylic acid					
	557.2	15.82	0	28.38	51.9	15.82	28.9
		2*A14+4*A15+4*A19+2*A117+2*A10					[216]
$C_{10}H_4Cl_2O_2$		2,3-dichloro-1,4-naphthalenedione					
	469	28.53	0	60.83	54.7	28.53	25.7
		A14+3*A15+4*A19+2*A114+2*A22*D22+4*A10					[215]
$C_{10}H_5Cl_4NO_2S$		3α,4,7,7α-tertrahydro-2-[(1,1,2,2-tetrachloroethyl)thio]-1H-isoindole-1,3(2H)-dione					
	432.7	40.22	0	92.96	81.4	40.22	35.2
		A14+2*A15+2*A19+A128+4*A10+A4*B4+A3*B3+4*A22+A84					[221]
$C_{10}H_5Cl_7$		1,4,5,6,7,8,8-heptachloro-3α,4,7,7α-tetrahydro-4,7-endo-methanoindene					
	358.2	23.4	65.33				
	371	2.09	5.63	70.96	41.5	25.49	15.4
		3*A14+A15+3*A17+2*A19+7*A22*G22+2*A18+3*A116					[222]
$C_{10}H_5Cl_{17}O$		1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3α,4,7,7α-tetrahydro-4,7-endo-methanoindan					
	385.2	18.9	49.07				
	434.9	2.85	6.55	55.62	42.4	21.75	18.5
		4*A14−A15+3*A17+2*A19+7*A22*G22+5*A16+A112					[222]
$C_{10}H_6Cl_8$		1,2,4,5,6,7,8,8-octachloro-2,3,3α,4,7,7α-hexahydro-4,7-methano-1H-indene					
	379.88	23.15	0	60.94	46.1	23.15	17.5
		3*A14+A15+3*A17+2*A19+2*A16+2*A16+8*A22*G22					[221]
$C_{10}H_6Cl_4O_4$		dimethyl-2,3,5,6-tetrachloro-1,4-benzenedicarboxylate					
	431.7	30.23	0	70.01	70.3	30.23	30.4
		6*A12+4*A22*F22+2*A38+2*A1					[215]
$C_{10}H_6OS_2$		naphthalene 1,8-disulfide S-oxide					
	363	3.2	8.8				
	421.2	23.3	0	55.32	42.9	23.3	18.1
		A14+2*A15+2*A19+A19+6*A10+A12+A133					[176]
$C_{10}H_6S_2$		naphthalene disulfide					
	394.8	13	0	32.93	34.6	13	13.7
		A14+2*A15+3*A19+6*A10+A12+A132					[44]
$C_{10}H_7Br$		1-bromonaphthalene					
	271.4	15.16	0	55.86	47.0	15.16	12.8
		7*A10+3*A12+A21					[83]
$C_{10}H_7Br$		2-bromonaphthalene					
	319	5.77	18.09				
	329	14.40	43.76	61.85	47.0	20.17	15.5
		7*A10+2*A12+A12+A21					[216]
$C_{10}H_7Cl$		1-chloronaphthalene					
	270.7	12.9	0	47.65	40.2	12.9	10.9
		7*A10+3*A12+A22					[83]
$C_{10}H_7Cl$		2-chloronaphthalene					
	332	14.7	0	44.28	40.2	14.7	13.4
		7*A10+3*A12+A22					[83]
$C_{10}H_7Cl_5O$		2-(3,5-dichlorophenyl)-2(2,2,2-trichloroethyl)oxirane					
	313.2	18.54	0	59.17	62.9	18.54	19.7
		A14+2*A12+A11+3*A10+A17+A112+5*A22*F22+A2+A4*B4					[221]
$C_{10}H_7I$		1-iodonaphthalene					
	280	15.91	0	56.82	48.8	15.91	13.7
		7*A10+3*A12+A29					[215]
$C_{10}H_7I$		2-iodonaphthalene					
	327.6	16.04	0	48.96	48.8	16.04	16.0
		7*A10+3*A12+A29					[215]
$C_{10}H_7NO_2$		1-nitronaphthalene					
	329.9	18.43	0	55.87	47.2	18.43	15.6
		7*A10+3*A12+A50					[215]
$C_{10}H_8$		naphthalene					
	353.4	19.1	0	53.75	44.4	19.1	15.7
		8*A10+2*A12					[215]
$C_{10}H_8$		azulene					

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	373.5	17.53	0	46.9	44.2	17.53	16.5
		2*A14+4*A15+2*A19+8*A18					[244]
$C_{10}H_8ClN_3O$		5-amino-4-chloro-2-phenyl-3(2H)-pyridazinone					
	479.2	26.75	0	55.83	62.8	26.75	30.1
		A14+3*A15+2*A19+A18*B18+A45+A22*D22+A125					[215]
		+5*A10+A12+A118					
$C_{10}H_8ClN_3O_2$		4-(2-chlorophenylhydrazone)-3-methyl-5-isoxazolone					
	440.4	28.04	0	63.66	61.3	28.04	27.0
		A14+2*A15+2*A19+A115+A118+A42+A1+4*A10+2*A12+A44+A22*E22					[221]
$C_{10}H_8O$		α-napthol					
	369	23.01	0	62.34	49.7	23.01	18.4
		7*A10+2*A12+A31+A12					[215]
$C_{10}H_8O$		β-napthol					
	393.6	18.79	0	47.7	49.7	18.79	19.6
		7*A10+2*A12+A31+A12					[215]
$C_{10}H_8O_3$		4-methyl-7-hydroxycoumarin					
	460.7	29.14	0	63.25	60.3	29.14	27.8
		A14+3*A15+A115+A31+3*A19+A18*B18+3*A10+A12+A1					[216]
$C_{10}H_9Cl_2NO$		N-(3,4-dichlorophenyl)-2-methyl-2-propenamide					
	395.5	32.04	0	81.0	57.8	32.04	22.9
		A1+A5+A7+3*A10+3*A12+2*A22*C22+A60					[215]
$C_{10}H_9Cl_3O_3$		methyl 2-(2,4,5-trichlorophenoxy)propionate					
	360.6	31.95	0	88.59	71.3	31.95	25.7
		2*A10+4*A12+2*A1+A3*B3+A32+A38+3*A22*E22					[215]
$C_{10}H_9Cl_3O_3$		4-(2,4,5-trichlorophenoxy)butanoic acid					
	386.7	30.28	0	78.3	89.6	30.28	34.6
		2*A10+4*A12+3*A22*E22+A36*E36+A32+3*A2					[215]
$C_{10}H_9Cl_4NO_2S$		N-[(1,1,2,2-tetrachloroethyl)thio]-4-cyclohexene-1,2-dicarboximide					
	432	43.1	0	99.76	80.5	43.1	34.8
		2*A14+3*A15+2*A16+2*A18+A128+A4*B4+A3*B3+4*A22*G22+A84					[232]
$C_{10}H_9N$		1-naphthylamine					
	323.2	15.53	0	48.05	50.8	15.53	16.4
		7*A10+2*A12+A45+A12					[215]
$C_{10}H_9N$		2-naphthylamine					
	386.2	23.33	0	60.38	50.8	23.33	19.6
		7*A10+2*A12+A45+A12					[215]
$C_{10}H_9NO_2$		4-methyl-7-aminocoumarin					
	499.9	32.09	0	64.19	61.4	32.09	30.7
		A14+3*A15+A115+A45+3*A19+A18*B18+3*A10+A12+A1					[216]
$C_{10}H_{10}$		bullvalene					
	366.5	15.25	0	41.61	35.3	15.25	12.9
		3*A14+A15+4*A16+6*A18					[216]
$C_{10}H_{10}Cl_2O_3$		4-(2,4-dichlorophenoxy)butyric acid					
	391.4	38.42	0	98.16	88.3	38.42	34.6
		3*A10+3*A12+3*A2+A36*D36+2*A22*D22+A32					[215]
$C_{10}H_{10}O_3$		2,3-dihydro-2,2-dimethyl-7-benzofuranol-3-one					
	440.6	21.79	0	49.47	49.6	21.79	21.9
		A14+2*A15+2*A19+A17+A112+A114+2*A1+A31+3*A10+A11					[221]
$C_{10}H_{10}O_4$		1,2-dicarbomethoxybenzene					
	274.2	16.95	0	61.92	65.2	16.95	17.9
		4*A10+2*A38+2*A12+2*A1					[217]
$C_{10}H_{10}O_4$		1,3-dicarbomethoxybenzene					
	341.2	25.3	0	74.15	65.2	25.3	22.3
		4*A10+2*A38+2*A12+2*A1					[217]
$C_{10}H_{10}O_4$		1,4-dicarbomethoxybenzene					
	413.8	32.09	0	77.55	65.2	32.09	27.0
		4*A10+2*A38+2*A12+2*A1					[217]
$C_{10}H_{11}ClO_3$		(*dl*) 2-(2-chloro-3-methylphenoxy)propionic acid					
	391.5	30.54	0	78.02	73.9	30.54	29.0
		3*A10+2*A1+A3*B3+2*A12+A11+A32+A36*C36+A22*C22					[273]
$C_{10}H_{11}ClO_3$		(D) 2-(2-chloro-3-methylphenoxy)propionic acid					
	359.5	22.18	0	61.68	73.9	22.18	26.6
		3*A10+2*A1+A3*B3+2*A12+A11+A32+A36*C36+A22*C22					[273]
$C_{10}H_{11}F_3N_2O$		N,N-dimethyl-N′-[3-(trifluoromethyl)-phenyl]urea					
	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)
$C_{10}H_{11}F_3N_2O_3S$		N-[4-methyl-3-[[(trifluoromethyl)sulfonyl]amino]phenyl]acetamide					
	455.7	40.47	0	88.81	57.9	40.47	20.4
		2*A1+3*A10+A11+2*A12+A4*B4+3*A25+A95+A60					[221]
$C_{10}H_{11}NO_3$		N-salicylidene-β-alanine					
	408	28.5	0	69.85	81.4	28.5	33.2
		2*A2+A36*C36+4*A10+2*A12+A31+A6*B6+A42					[216]
$C_{10}H_{12}$		1,2,3,4-tetrahydronaphthalene					
	237.4	12.45	0	52.44	49.6	12.45	11.8
		A14+3*A15+4*A10+2*A19					[216]
$C_{10}H_{12}$		*endo*-dicyclopentadiene					
	216	9.66	44.72				
	304.8	2.22	7.28	52.01	38.5	11.88	11.7
		3*A14+A15+4*A16+4*A18					[216]
$C_{10}H_{12}ClNO_2$		isopropyl-3-chlorophenylcarbamate					
	313.9	17.75	0	56.55	67.0	17.75	21.0
		2*A1+A3*B3+4*A10+2*A12+A69+A22*B22					[215]
$C_{10}H_{12}ClN_3O_2$		5-chloro-6-[[[(methylamino)carbonyl]oxy]imino]bicyclo[2.2.1]heptane-2-carbonitrile					
	431.6	26.07	0	60.4	59.6	26.07	25.7
		2*A14+A15+A56+A22*D22+2*A16+2*A16+A19+A42+A69+A1					[221]
$C_{10}H_{12}N_2O_3$		allobarbitiol					
	442.6	32.31	0	73	73.4	32.31	32.5
		A14+3*A15+A129+A124+A17+2*A2+2*A5+2*A6					[241]
$C_{10}H_{12}N_2O_3$		2-ethoxyisonitrosoacetanilide					
	405	23	0	56.79	63.0	23	25.5
		A1+A2+4*A10+2*A12+A32+A60+A53+A6*B6					[216]
$C_{10}H_{12}N_2O_3$		4-ethoxyisonitrosoacetanilide					
	490	7.6	0	15.51	63.0	7.6	30.9
		A1+A2+4*A10+2*A12+A32+A60+A53+A6*B6					[216]
$C_{10}H_{12}N_2O_3S$		3-(1-methylethyl)-(1H)-2,1,3-benzothiadiazin-4(3H)-one 2,2-dioxide					
	412.5	21.77	0	52.76	53.0	21.77	21.9
		A14+3*A15+2*A19+A125+4*A10+2*A1+A3*B3+A137					[221]
$C_{10}H_{12}N_2O_5$		2-sec-butyl-4,6-dinitrophenol					
	313.7	21.81	0.	69.54	64.4	21.81	20.2
		2*A10+A11+3*A12+2*A1+A2+A3+2*A50+A31					[221]
$C_{10}H_{12}N_2S$		N-allyl-N-phenylthiourea					
	375	27.61	0	73.64	73.7	27.61	27.6
		5*A10+A12+A2+A5+A6+A90					[216]
$C_{10}H_{12}N_3O_3PS_2$		S-(3,4-dihydro-4-oxobenzo[*d*][1,2,3]-triazin-3-ylmethyl) O,O-dimethylphoshorodithioate					
	345.3	27.76	0	80.4	61.6	27.76	21.3
		A14+3*A15+2*A118+2*A19+4*A10+A125+A2+2*A1+A80					[215]
$C_{10}H_{12}O_2$		4-propylbenzoic acid					
	301	3.4	11.3				
	422	23.3	55.21	66.51	57.8	26.7	24.4
		A1+2*A2+A11+A12+4*A10+A36					[177]
$C_{10}H_{12}O_3$		(*dl*) 3-hydroxy-3-phenylbutyric acid					
	330	19.66	0	59.59	63.6	19.66	21.0
		A1+A2+A4*B4+5*A10+A11+A36*B36+B30*A30					[220]
$C_{10}H_{12}O_3$		(*d*) 3-hydroxy-3-phenylbutyric acid					
	357	22.59	0	63.29	63.6	22.59	22.7
		A1+A2+A4*B4+5*A10+A11+B36*A36+B30*A30					[220]
$C_{10}H_{12}O_3$		4-ethoxyphenylacetic acid					
	360.2	23	0	63.85	65.2	23	23.5
		4*A10+A11+A12+2*A2+A1+A36*B36+A32					[215]
$C_{10}H_{12}O_3$		4-methoxyphenylpropionic acid					
	376.9	28.5	0	75.62	65.2	28.5	24.6
		4*A10+A11+A12+2*A2+A1+A36*B36+A32					[215]
$C_{10}H_{12}O_3$		propyl 4-hydroxybenzoate					
	369.2	27.99	0	75.82	74.5	27.99	27.5
	369.8	26.7	0	72.3	74.5	26.7	27.5
		A1+2*A2+4*A10+2*A12+A31+A38					[218, 395]
$C_{10}H_{13}ClN_2O_2$		N′-(3-chloro-4-methoxyphenyl)-N,N-dimethylurea					
	399.2	27.48	0	68.86	68.7	27.48	27.5
		3*A1+3*A10+3*A12+A22*C22+A32+A64*C64					[221]
$C_{10}H_{13}ClN_6$		2-((4-chloro-6-(cyclopropylamino)-1,3,5-triazin-2-yl)amino-2-methylpropanenitrile					
	438.5	22.51	0	51.34	64.6	22.51	28.3
		A14+A16+3*A41+3*A12+A22*F22+2*A44+2*A1+A56+A4*B4					[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)
$C_{10}H_{13}ClO_3$		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]
$C_{10}H_{13}NO_2$		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]
$C_{10}H_{13}NO_2$		methyl *p*-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]
$C_{10}H_{13}NO_2$		*p*-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]
$C_{10}H_{13}NO_2$		propyl N-phenyl carbamate					
	331	21.08	0	63.68	72.0	21.08	23.9
		2*A2+A1+5*A10+A12+A69					[102]
$C_{10}H_{13}NO_2$		isopropyl phenylcarbamate					
	359.5	19.37	0	53.88	65.7	19.37	23.62
		5*A10+A12+2*A1+A3*B3+A69					[215]
$C_{10}H_{13}NO_2$		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]
$C_{10}H_{13}NO_4$		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]
$C_{10}H_{13}N_5O_3$		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					
$C_{10}H_{13}N_5O_3$		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					
$C_{10}H_{13}N_5O_4$		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					
$C_{10}H_{13}N_5O_4$		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					
$C_{10}H_{14}$		*tert*-butylbenzene					
	215	8.40	0	39.1	45.4	8.40	9.8
		3*A1+A4+5*A10+A11					[216]
$C_{10}H_{14}$		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]
$C_{10}H_{14}$		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]
$C_{10}H_{14}$		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]
$C_{10}H_{14}$		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]
$C_{10}H_{14}$		*n*-butylbenzene					
	185.3	11.22	0	60.56	66.5	11.22	12.3
		5*A10+A1+3*A2+A11					[216]
$C_{10}H_{14}Cl_2NO_2PS$		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]
$C_{10}H_{14}NO_5PS$		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]
$C_{10}H_{14}N_4O_2$		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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{10}H_{14}N_4O_2$		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]
$C_{10}H_{14}N_6O$		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]
$C_{10}H_{14}O$		4-*tert*-butylphenol					
	373.2	14.52	0	38.9	50.7	14.52	18.9
		3*A1+A4+4*A10+A11+A12+A31					[101]
$C_{10}H_{14}O$		thymol					
	324.2	22.01	0	67.88	52.2	22.01	16.9
		3*A10+2*A11+A12+3*A1+A3+A31					[220]
$C_{10}H_{14}O_2$		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]
$C_{10}H_{14}O_3$		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]
$C_{10}H_{14}O_3$		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]
$C_{10}H_{14}O_8$		(*dl*) dimethyl diacetyltartrate					
	355.2	25.94	0	73.03	81.4	25.94	28.9
		4*A1+2*A3*B3+4*A38					[226]
$C_{10}H_{14}O_8$		(*d*) dimethyl diacetyltartrate					
	377.2	29.29	0	77.65	81.4	29.29	30.7
		4*A1+2*A3*B3+4*A38					[226]
$C_{10}H_{14}Si$		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]
$C_{10}H_{14}Si$		vinyldimethylphenylsilane					
	190.7	12.26	0	64.28	58.9	12.26	11.2
		2*A1+A5+A6*B6+5*A10+A12+A109					[216]
$C_{10}H_{15}Br$		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]
$C_{10}H_{15}Cl$		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]
$C_{10}H_{15}I$		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]
$C_{10}H_{15}N_5$		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]
$C_{10}H_{15}NO$		(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]
$C_{10}H_{15}NO$		(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]
$C_{10}H_{16}$		tricyclo[5.2.1.$0^{2,6}$]decane					
	352	2.95	0	8.38	0	2.95	0
		No prediction made					[216]
$C_{10}H_{16}$		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]
$C_{10}H_{16}Cl_3NOS$		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)	
		$A5+A7+A4*B4+4*A1+2*A3*B3+3*A22*C22+A93$						[215]
$C_{10}H_{16}NO_4PS$		O-[4-(dimethylamino)sulfonyl]phenyl] O,O-dimethyl phosphorothionate						
	326.8	26.5	0	81.08	74.8	26.5	24.5	
		$A94+4*A1+A79+4*A10+2*A12$						[221]
$C_{10}H_{16}N_2$		ethyl(1,1-dimethylpropyl)malononitrile						
	307.5	19.25	0	62.59	62.4	19.25	19.2	
		$4*A1+2*A2+A4+A4*B4+2*A56$						[245]
$C_{10}H_{16}N_4O_2S$		3-(5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl)-4-hydroxy-1-methyl-2-imidazolidinone						
	408.9	25.46	0	62.26	62.2	25.46	25.5	
		$2*A14+4*A15+A127+A16+4*A1+A4+2*A19+A131+2*A118+A30*E30$						[221]
$C_{10}H_{16}O$		(D) camphor						
	242	16.0	66.1					
	374	0.23	0.62					
	452	5.3	11.7	78.5	38.0	21.5	17.2	
		$A114+2*A14+A15+A17+A17+A16+3*A1$						[45]
$C_{10}H_{16}O_2$		1,6-cyclodecanedione						
	372.2	29.58	0	79.5	56.6	29.58	21.1	
		$A14+7*A15+2*A114$						[114]
$C_{10}H_{16}O_4$		1,4-cyclohexanedione *bis* ethylene ketal						
	353.2	25.77	0	72.97	54.4	25.77	19.2	
		$3*A14+5*A15+4*A112+2*A17$						[114]
$C_{10}H_{17}NO$		D camphor oxime						
	383	13.3	34.73					
	389	1.8	4.63	39.35	40.6	15.1	15.8	
		$2*A14+A15+A16+A17+A17+3*A1+A53+A19$						[45]
$C_{10}H_{17}NO$		DL camphor oxime						
	375	3	8					
	380	11.2	29.47					
	388	1.2	3.09	40.57	40.6	15.4	15.8	
		$2*A14+A15+A16+A17+A17+3*A1+A53+A19$						[45]
$C_{10}H_{17}N_5O$		6-methoxy-N,N′-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine						
	363.5	21.18	0	58.26	73.0	21.18	26.5	
		$5*A1+2*A3*B3+A32+3*A41+3*A12+2*A44$						[215]
$C_{10}H_{18}$		*cis*-decalin						
	242.8	14.43	0	59.45	52.1	14.43	12.65	
		$2*A14+4*A15+2*A16$						[216]
$C_{10}H_{18}$		*trans*-decalin						
	216.1	2.13	9.87					
	230.2	9.49	41.22	51.1	52.1	11.62	11.99	
		$2*A14+4*A15+2*A16$						[216]
$C_{10}H_{18}N_5S$		N-(1,1-dimethylethyl)-N′-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine						
	375.9	21.42	0	56.99	74.0	21.42	27.8	
		$5*A1+A2+A4*B4+2*A44+3*A41+3*A12+A84$						[221]
$C_{10}H_{18}N_6O_2$		1-(sarcosine)-3,5-bis(dimethylamino)-*s*-triazine						
	431	29.83	0	69.33	68.6	29.83	29.6	
		$5*A1+3*A41+3*A12+3*A43+A36*F36+A2$						[242]
$C_{10}H_{18}O_4$		sebacic acid						
	404	40.8	0	101.0	106.9	40.8	43.2	
		$8*A2*B2+2*A36*B36$						[216]
$C_{10}H_{18}Si$		5-trimethylsilyl-2-norbornene						
	201.6	6.84	0	33.93	78.4	6.84	15.81	
		$2*A14+A14+3*A16+2*A18+3*A1+A109$						[162]
$C_{10}H_{20}$		*n*-butylcyclohexane						
	198.4	14.14	0	71.28	68.7	14.14	13.6	
		$A14+A1+A16+3*A2+3*A15$						[216]
$C_{10}H_{20}$		1-decene						
	198.3	7.95	40.09					
	206.9	13.81	66.73	106.8	105.5	21.76	21.8	
		$A1+7*A2*B2+A5+A6$						[216]
$C_{10}H_{20}$		2,2,5,5-tetramethylhex-3-ene						
	235.8	1.21	5.13					
	243.5	4.33	17.78					
	268.9	10.25	38.12	61.03	46.3	15.79	12.5	
		$6*A1+2*A4+2*A6$						[42]
$C_{10}H_{20}N_6$		1-(ethylmethylamino)-3,5-bis(dimethylamino)-*s*-triazine						
	384	21.3	0	55.46	56.3	21.3	21.6	
		$3*A41+3*A12+2*A43+6*A1+A44+A3*B3$						[215]
$C_{10}H_{20}O$		(*dl*) menthol						

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)
	301.2	10.25	0	34.03	38.4	10.25	11.6
		3*A1+A14+3*A15+2*A16+A30+A3+A16					[226]
$C_{10}H_{20}O$		(*l*) menthol					
	316.2	11.88	0	37.58	38.4	11.88	12.1
		3*A1+A14+3*A15+2*A16+A30+A3+A16					[226]
$C_{10}H_{20}O$		decanal					
	268.2	30.6	0	114.1	113.8	30.6	30.5
		8*A2*B2+A1+A34					[93]
$C_{10}H_{20}O_2$		decanoic acid					
	304.5	27.99	0	91.28	105.6	27.82	32.2
		8*A2*B2+A1+A36					[216]
$C_{10}H_{22}$		*n*-decane					
	243.5	28.7	0	117.99	109.8	28.7	26.7
		2*A1+8*A2*B2					[216]
$C_{10}H_{22}$		5-methylnonane					
	186.7	16.65	0	89.19	79.2	16.65	14.8
		3*A1+6*A2+A3					[216]
$C_{10}H_{22}$		(DL) 4-methylnonane					
	174.7	15.19	0	86.94	79.2	15.19	13.8
		3*A1+6*A2+A3					[216]
$C_{10}H_{22}$		(DL) 3-methylnonane					
	188.5	18.7	0	99.22	92.4	18.7	17.4
		3*A1+6*A2*B2+A3					[216]
$C_{10}H_{22}$		2-methylnonane					
	198.8	17.49	0	87.97	92.4	17.49	18.4
		3*A1+6*A2*B2+A3					[216]
$C_{10}H_{22}O_2$		1,10-decanediol					
	345.5	41.7	0	120.69	129.5	41.7	44.8
		10*A2*B2+2*A30*B30					[215]
$C_{10}H_{22}O_2S$		3(*n*-heptylthio)-1,2-propanediol					
	289.5	27.3	94.3				
	292.5	1.7	5.81	100.11	114.3	29.0	33.4
		A1+6*A2*B2+A84+2*A30*C30+A3*B3+2*A2					[217]
$C_{10}H_{22}O_3$		3(*n*-heptyloxy)-1,2-propanediol					
	288	28.8	100				
	246.2	1	4.06	104.06	116.9	29.8	28.8
		A1+6*A2*B2+A32+2*A30*C30+A3*B3+2*A2					[217]
$C_{10}H_{22}S$		1-decanethiol					
	247.9	33.3	0	134.31	124.6	33.3	30.9
		9*A2*B2+A1+A86					[216]
$C_{10}H_{23}NO_2$		3(*n*-heptylamino)-1,2-propanediol					
	324.9	28.8	0	88.64	106.9	28.8	34.7
		A1+6*A2*B2+A44+2*A30*C30+A3*B3+2*A2					[217]
$C_{10}H_{26}O_3Si_3$		1,1,3,3-tetraethyl-5,5-dimethylcyclotrisiloxane					
	195	0.13	0.67				
	260	9.52	36.62	37.29	78.1	9.65	20.3
		6*A1+4*A2+3*A112+3*A139+A14+3*A15					[216]
$C_{11}H_8O_2$		1-naphthoic acid					
	435.2	19.89	0	45.7	42.8	19.89	18.6
		7*A10+2*A12+A36+A12					[215]
$C_{11}H_8O_2$		2-naphthoic acid					
	460.2	23.54	0	51.15	42.8	23.54	19.7
		7*A10+2*A12+A36+A12					[215]
$C_{11}H_9Cl_2NO_2$		4-chlorobut-2-ynyl 3-chlorophenylcarbamate					
	344.1	26.91	0	78.21	66.4	26.91	22.9
		4*A10+2*A12+2*A2+2*A9+2*A22*C22+A69					[221]
$C_{11}H_{10}$		1-methylnaphthalene					
	240.7	4.98	20.69				
	242.7	6.95	28.62	49.3	44.9	11.92	10.9
		A1+7*A10+A11+2*A12					[216]
$C_{11}H_{10}$		2-methylnaphthalene					
	288.5	5.61	19.43				
	307.4	12.13	39.43	58.87	44.9	17.74	13.8
		A1+7*A10+A11+2*A12					[216]
$C_{11}H_{10}O_2$		2-acetyl-1-naphthol					
	371.8	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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{11}H_{10}O_2$		1-acetyl-2-naphthol					
	337	21.34	0	63.32	57.0	21.34	19.2
		6*A10+4*A12+A31+A35+A1					[215]
$C_{11}H_{10}O_4$		*p*-methacryloyloxybenzoic acid					
	455	34	0	74.73	62.7	34	28.5
		4*A10+2*A12+A36*B36+A38+A5+A7+A1					[216]
$C_{11}H_{11}Cl_3O_3$		methyl 2-(2,4,5-trichlorophenoxy)butyrate					
	316.5	28.87	0	91.22	78.3	28.87	24.8
		3*A22*E22+2*A1+4*A12+2*A10+A38+A32+A2+A3*B3					[232]
$C_{11}H_{12}NO_3PS$		O,O-dimethyl S-phthalimidomethyl phosphorodithioate					
	343.2	26.96	0	78.56	79.7	26.96	27.3
		A14+2*A15+A128+2*A19+4*A10+2*A1+A2+A80					[221]
$C_{11}H_{12}Cl_2O_3$		methyl 4-(2,4-dichlorophenoxy)butyrate					
	309.6	32.64	0	105.41	83.5	32.64	25.9
		2*A22*D22+A1+3*A12+3*A10+A38+A32+3*A2					[232]
$C_{11}H_{13}F_3N_2O_3S$		5′-(trifluoromethanesulphonamide)acet-2′,4-xylidide					
	457.3	37.66	0	82.35	61.6	37.66	28.1
		3*A1+2*A10+2*A11+2*A12+A60+A4*B4+3*A25+A95					[221]
$C_{11}H_{13}ClO_3$		4-(4-chloro-2-methylphenoxy)butanoic acid					
	373.5	32.02	0	85.73	87.6	32.02	32.7
		3*A10+2*A12+A11+A1+3*A2+A36*C36+A22*C22+A32					[221]
$C_{11}H_{13}NO_4$		2,3-diisopropylidenedioxyphenyl-N-methylcarbamate					
	402.6	29.45	0	73.14	62.2	29.45	25.1
		A14+2*A15+2*A19+2*A112+A17+3*A1+A69+3*A10+A12					[221]
$C_{11}H_{13}F_3N_4O_4$		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
		4*A12+A10+A11+3*A25+A4*B4+2*A50+A45+A43+2*A1+2*A2					[221]
$C_{11}H_{14}$		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
		5*A14−4*A15+8*A16					[183]
$C_{11}H_{14}$		1,1-dimethylindan					
	227.4	11.99	0	52.73	46.5	11.99	10.6
		A14+2*A15+A17+A1*2+2*A19+4*A10					[216]
$C_{11}H_{14}$		4,6-dimethylindan					
	256.5	12.88	0	50.21	47.0	12.88	12.1
		A14+2*A15+2*A19+2*A11+2*A10+2*A1					[216]
$C_{11}H_{14}$		4,7-dimethylindan					
	272.7	13.52	0	49.58	47.0	13.52	12.8
		A14+2*A15+2*A19+2*A11+2*A10+2*A1					[216]
$C_{11}H_{14}ClNO$		2-chloro-N-isopropyl N-phenylacetamide					
	351.4	26.05	0	74.13	67.2	26.05	23.6
		5*A10+A12+2*A1+A3*B3+A2+A22*B22+A59					[221]
$C_{11}H_{14}O_2$		4-*tert*-butylbenzoic acid					
	440	17.91	0	40.7	43.8	17.91	19.3
		4*A10+A11+A12+A36+3*A1+A4					[217]
$C_{11}H_{14}O_3$		(*dl*) 3-phenyl-3-hydroxy-2,2-dimethylpropanoic acid					
	407	37.24	0	91.49	64.3	37.24	26.1
		5*A10+A11+A3*B3+A4*B4+2*A1+B30*A30+A36*B36					[220]
$C_{11}H_{14}O_3$		(*d*) 3-phenyl-3-hydroxy-2,2-dimethylpropanoic acid					
	431	39.75	0	92.22	64.3	39.45	27.7
		5*A10+A11+A3*B3+A4*B4+2*A1+B30*A30+A36*B36					[220]
$C_{11}H_{14}O_3$		4-methoxyphenylbutyric acid					
	330.9	25.3	0	76.46	72.4	25.3	24.0
		4*A10+A11+A12+3*A2+A1+A36*B36+A32					[233]
$C_{11}H_{14}O_3$		(*dl*) 3-hydroxy-3-phenylvaleric acid					
	394	35.15	0	89.2	70.7	35.15	27.9
		5*A10+A11+A1+2*A2+A4*B4+B36*A36+B30*A30					[220]
$C_{11}H_{14}O_3$		(*d*) 3-hydroxy-3-phenylvaleric acid					
	379	30.96	0	81.69	70.7	30.96	26.8
		5*A10+A11+A1+2*A2+A4*B4+A36*B36+B30*A30					[220]
$C_{11}H_{15}N$		1-cyanoadamantane					
	280	5.5	19.64				
	458	15	32.75	52.39	42.8	20.5	19.6
		3*A14+A15+3*A16+A17+A56					[148]
$C_{11}H_{15}NO_2$		4-*trans*-cyanocyclohexyl (E) 2-butenoate					

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)
	366.2	24.4	0	66.63	67.2	24.4	24.6
		A14+3*A15+2*A16+A56+A38+A1+A6*B6+A6					[140]
$C_{11}H_{15}NO_2$		butyl 4-aminobenzoate					
	331.1	20.46	0	61.79	82.7	20.46	27.4
		4*A10+2*A12+A1+A45+A38+3*A2					[215]
$C_{11}H_{15}NO_2$		2-(1-methyllethyl)phenyl methylcarbamate					
	369.3	26.14	0	70.78	59.6	26.14	22.0
		3*A1+A3+4*A10+A11+A12+A69					[221]
$C_{11}H_{15}NO_2$		4-methylthio-3,5-xylyl methylcarbamate					
	393.8	30.36	0	77.11	63.7	30.36	25.1
		4*A1+2*A11+2*A12+A69+A84+2*A10					[215]
$C_{11}H_{15}NO_3$		1,2-dihydro-6-neopentyl-2-oxonicotinic acid					
	469.2	19.33	0	41.2	60.6	19.33	28.4
		A14+3*A15+A124+2*A18+2*A19+A36+3*A1+A2+A4					[164]
$C_{11}H_{15}N_3O_2$		N-caproyl-pyrazinamide					
	351.7	35.95	0	102.22	90.4	35.95	31.8
		A1+4*A2+3*A10+A12+2*A41+A71					[9]
$C_{11}H_{16}$		pentamethylbenzene					
	296.8	1.98	6.67				
	328.2	10.67	32.51	39.33	47.3	12.65	15.5
		5*A1+A10+5*A11					[216]
$C_{11}H_{16}N_4O_2$		8-butyltheophylline					
	509.2	32.3	0	63.43	74.5	32.3	37.9
		2*A14+3*A15+2*A125+A118+A121+3*A1+3*A19+3*A2					[236]
$C_{11}H_{16}N_4O_2$		8-*tert*-butyltheophylline					
	402.3	48.2	0	119.81	53.4	48.2	21.5
		2*A14+3*A15+2*A125+A118+A121+2*A1+3*A19+3*A1+A4					[236]
$C_{11}H_{16}Si$		vinyldimethylbenzylsilane					
	204.1	11.6	0	56.83	65.3	11.6	13.3
		2*A1+A2+A109+5*A10+A11+A5+A6					[216]
$C_{11}H_{17}N_5$		6,9-dimethyl-8-butyladenine					
	409.2	36	0	87.98	75.8	36	31.0
		A14+2*A15+3*A19+3*A1+A118+A119+2*A41+A10+A12+A44+3*A2					[240]
$C_{11}H_{18}$		1-methyladamantane					
	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
		3*A14+A15+3*A16+A17+A1					[146]
$C_{11}H_{19}NO_3$		2-isopropoxyphenyl N-methylcarbamate					
	363.1	22.96	0	63.23	72.9	22.96	26.5
		3*A1+A69+A3*B3+4*A10+2*A12+A32					[215]
$C_{11}H_{19}NS$		2,4-di-*tert*-butylthiazole					
	258.2	10.5	0	40.67	52.4	10.5	13.5
		A14+2*A15+2*A19+A18*B18+6*A1+2*A4+A131+A118					[61]
$C_{11}H_{19}N_3O$		5-butyl-2-ethylamino-6-methylpyrimidin-4-ol					
	432.5	20.32	0	46.98	83.9	20.32	36.3
		2*A11+2*A12+3*A1+3*A2+A44+A31+2*A41+A2					[215]
$C_{11}H_{19}N_5S$		6-ethylthio-N,N′-*bis*(1-methylethyl)1,3,5-triazine-2,4-diamine					
	377.7	23.94	0	63.38	77.2	23.94	29.2
		3*A41+3*A12+5*A1+2*A3*B3+A2+A84+2*A44					[215]
$C_{11}H_{20}N_6$		1-pyrrolidinyl-3,5-*bis*(dimethylamino)-*s*-triazine					
	403.1	25.61	0	63.53	57.6	25.61	23.2
		A14+2*A15+A119+4*A1+2*A43+3*A12+3*A41					[215]
$C_{11}H_{20}N_6O$		1-morpholinyl-3,5-*bis*(dimethylamino)-*s*-triazine					
	397.4	24.69	0	62.13	62.5	24.69	24.8
		A14+3*A15+A119+A112+4*A1+2*A43+3*A41+3*A12					[215]
$C_{11}H_{20}N_7S$		1-(thiomorpholinyl-3,5-*bis*(dimethylamino)-*s*-triazine)					
	391.2	29.08	0	74.33	64.2	29.08	25.1
		4*A1+2*A43+3*A41+3*A12+A14+3*A15+A119+A131					[215]
$C_{11}H_{20}O_2$		undecanolactone					
	250.2	3.36	13.43				
	275.3	12.61	45.8	59.23	69.8	15.97	19.2
		A14+9*A15+A115					[216]
$C_{11}H_{20}O_4$		undecanedioic acid					
	385	39.65	0	102.99	116.2	39.65	44.7
		9*A2*B2+2*A36*B36					[216]
$C_{11}H_{21}N_5S$		6-(ethylthio)-N,N′-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine					

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)
	377.7	23.94	0	63.39	77.2	23.94	29.2
		5*A1+A2+2*A3*B3+3*A41+2*A44+A84+3*A12					[221]
$C_{11}H_{21}N_7$		1-(piperizinyl)-3,5-*bis*(dimethylamino)-*s*-triazine					
	382	23.01	0	60.24	63.5	23.01	24.3
		4*A1+2*A43+3*A41+3*A12+A14+3*A15+A119+A121					[215]
$C_{11}H_{22}$		1-undecene					
	217.3	9.2	42.36				
	224	16.99	75.84	118.2	114.8	26.19	25.7
		A1+8*A2*B2+A5+A6					[216]
$C_{11}H_{22}O$		2-undecanone					
	290.5	28.78	0	99.07	114.4	28.78	33.2
		2*A1+8*A2*B2+A35					[21]
$C_{11}H_{22}O_2$		undecanoic acid					
	290	8.13	28.03				
	301.6	25.98	86.15	114.22	114.9	34.11	34.7
		9*A2*B2+A1+A36					[216]
$C_{11}H_{24}$		*n*-undecane					
	236.6	6.86	29				
	247.6	22.18	89.6	118.6	119.1	29.03	29.5
		2*A1+9*A2*B2					[216]
$C_{11}H_{24}$		2-methyldecane					
	224.3	25.06	0	111.73	101.7	25.06	22.8
		3*A1+7*A2*B2+A3					[216]
$C_{11}H_{24}O$		methyl *n*-decyl ether					
	243.5	31.71	0	130.12	123.8	31.71	30.2
		2*A1+9*A2*B2+A32					[216]
$C_{11}H_{24}O_2S$		3(*n*-octylthio)-1,2-propanediol					
	306.5	39.8	0	129.85	123.4	39.8	37.8
		A1+7*A2*B2+A84+2*A30*C30+A3*B3+2*A2					[217]
$C_{11}H_{24}O_3$		3(*n*-octyloxy)-1,2-propanediol					
	296.1	33.4	0	112.8	126.0	33.4	37.3
		A1+7*A2*B2+A32+2*A30*C30+A3*B3+2*A2					[217]
$C_{11}H_{25}NO_2$		3(*n*-octylamino)-1,2-propanediol					
	335.9	45.1	0	134.27	116.0	45.1	39.0
		A1+7*A2*B2+A44+2*A30*C30+A3*B3+2*A2					[217]
$C_{12}Cl_{10}$		decachlorobiphenyl					
	577.7	39.34	0	68.1	72.1	39.34	41.6
		12*A12+10*A22*G22					[215]
$C_{12}F_{26}$		perfluorododecane					
	170.2	6.9	40.54				
	348.5	38.16	109.5	150.0	133.3	45.06	46.4
		12*A4*B4+6*A25+20*A26					[67]
$C_{12}HCl_9$		2,2′,3,3′,4,5,5′,6,6′-nonachlorobiphenyl					
	455.8	22.6	0	49.58	70.8	22.6	32.3
		11*A12+9*A22*G22+A10					[215]
$C_{12}H_2Cl_8$		2,2′,3,3′,5,5′,6,6′-octachlorobiphenyl					
	433.8	22.8	0	52.56	69.5	22.8	30.1
		10*A12+8*A22*G22+2*A10					[215]
$C_{12}H_3Cl_7$		2,2′,3,3′,5,5′,6-heptachlorobiphenyl					
	395.4	20.3	0	51.34	68.2	20.3	27.0
		9*A12+7*A22*G22+3*A10					[215]
$C_{12}H_4Cl_6$		2,2′,3,3′,5,5′-hexachlorobiphenyl					
	424.9	29.2	0	68.72	66.9	29.2	28.4
		6*A22*F22+4*A10+8*A12					[215]
$C_{12}H_4Cl_6$		2,2′,3,3′,6,6′-hexachlorobiphenyl					
	385.2	21.1	0	54.78	66.9	21.1	25.8
		6*A22*F22+4*A10+8*A12					[215]
$C_{12}H_4Cl_6$		2,2′,4,4′,6,6′-hexachlorobiphenyl					
	386.7	17.5	0	45.25	66.9	17.5	25.9
		6*A22*F22+4*A10+8*A12					[215]
$C_{12}H_5Cl_3O_2$		1,3,7-trichlorodibenzodioxin					
	421.7	30.8	0	73.04	61.0	30.8	25.7
		A14+3*A15+2*A112+3*A22*E22+4*A19+5*A10+3*A12					[20]
$C_{12}H_5Cl_5$		2,2′,4,5,5′-pentachlorobiphenyl					
	350.1	18.8	0	53.7	65.6	18.8	23.0
		5*A22*E22+5*A10+7*A12					[215]
$C_{12}H_5Cl_5$		2,3,4,5,6-pentachlorobiphenyl					

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)
	397.6	21.8	0	54.83	65.6	21.8	26.1
		5*A22*E22+5*A10+7*A12					[215]
$C_{12}H_6Cl_2O$		3,6-dichlorodibenzofuran					
	461.2	32.4	0	70.25	54.8	32.4	25.3
		A14+2*A15+2*A19+A19+A112+2*A22*C22+6*A10+2*A12					[20]
$C_{12}H_6Cl_4$		2,2′,4′,5-tetrachlorobiphenyl					
	339.1	23.4	0	69.01	64.3	23.4	21.8
		6*A12+6*A10+4*A22*D22					[215]
$C_{12}H_6Cl_4$		2,3,4,5-tetrachlorobiphenyl					
	363.9	25.2	0	69.25	64.3	25.2	23.4
		6*A12+6*A10+4*A22*D22					[215]
$C_{12}H_6Cl_4O_2S$		1,2,4-trichloro-5-((4-chlorophenyl)sulfonyl)benzene					
	419.9	28.94	71.21	68.92	64.6	28.94	27.1
		6*A12+6*A10+4*A22*E22+A88					[215]
$C_{12}H_6O_3$		1-8-naphthalic anhydride					
	542.3	23.32	0	43	47.0	23.32	22.5
		A14+3*A15+3*A19+A117+6*A10+A12					[221]
$C_{12}H_6S$		dibenzothiophene					
	373.2	21.6	0	57.74	53.9	21.6	20.1
		8*A10+A131+A14+2*A15+4*A19					[283]
$C_{12}H_7ClO_2$		1-chlorodibenzodioxin					
	378.2	23.2	0	61.34	58.5	23.2	22.1
		A14+3*A15+2*A112+4*A19+A12+7*A10+A22*C22					[20]
$C_{12}H_7ClO_2$		2-chlorodibenzodioxin					
	362.2	23.1	0	63.78	58.5	23.1	21.2
		A14+3*A15+2*A112+4*A19+A12+7*A10+A22*C22					[20]
$C_{12}H_7Cl_2NO_3$		2,4-dichlorophenyl 4-nitrophenyl ether					
	342	22.96	0	67.13	69.3	22.96	23.7
		7*A10+5*A12+2*A22*D22+A50+A32					[221]
$C_{12}H_7Cl_3$		2,4,6-trichlorobiphenyl					
	334.3	16.5	0	49.36	63.0	16.5	21.1
		5*A12+7*A10+3*A22*C22					[215]
$C_{12}H_7Cl_3$		2,4,5-trichlorobiphenyl					
	349.5	22.8	0	65.24	63.0	22.8	22.0
		5*A12+7*A10+3*A22*C22					[215]
$C_{12}H_8$		acenaphthylene					
	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
		A14+2*A15+3*A19+6*A10+A12+2*A16					[216,154]
$C_{12}H_8Br_2$		(*dl*) 1,2-dibromoacenaphthene					
	397	25.1	0	63.22	46.4	25.1	18.4
		6*A10+A14+2*A15+2*A21+2*A16+A12+3*A19					[273]
$C_{12}H_8Br_2$		(*d*) 1,2-dibromoacenaphthene					
	416	26.36	0	63.35	46.4	26.36	19.3
		6*A10+A14+2*A15+2*A21+2*A16+A12+3*A19					[273]
$C_{12}H_8Cl_2$		(*dl*) 1,2-dichloroacenaphthene					
	339	20.5	0	60.46	43.9	20.5	14.9
		2*A15+A14+6*A10+2*A22*B22+2*A16+3*A19					[273]
$C_{12}H_8Cl_2$		(*d*) 1,2-dichloroacenaphthene					
	375	21.34	0	56.9	43.9	21.34	16.5
		2*A15+A14+6*A10+2*A22*B22+2*A16+3*A19					[273]
$C_{12}H_8Cl_2$		2,6-dichlorobiphenyl					
	307.9	12.6	0	40.92	61.8	12.6	19.0
		4*A12+8*A10+2*A22*B22					[215]
$C_{12}H_8Cl_2O_2S$		4,4′-dichlorodiphenylsulphone					
	422	24.4	0	57.82	62.0	24.4	26.2
		8*A10+4*A12+2*A22*C22+A88					[216]
$C_{12}H_8Cl_2O_3S$		4-chlorophenyl 4-chlorobenzenesulfonate					
	360.0	23.63	0	65.64	69.7	23.63	25.1
		8*A10+4*A12+2*A22*C22+A89					[215]
$C_{12}H_8Cl_6O$		1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4α,5,6,7,8,8α-octahydro-1,4-endo, exo-5,8-dimethanonaphthalene (Dieldrin)					
	405.6	19.33	47.66				
	452.9	3.04	6.71	54.37	41.2	22.37	18.7
		5*A14−2*A15+6*A22*G22+3*A17+2*A19+4*A16+2*A16+A112					[222]
$C_{12}H_8Cl_6O$		1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4α,5,6,7,8,8α-octahydro-1,4-endo,					

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)
		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
		5*A14−2*A15+6*A22*G22+3*A17+2*A19+6*A16+A112					[222]
$C_{12}H_8N_2$		phenazine					
	450.2	20.92	0	46.47	51.2	20.92	23.1
		8*A10+4*A12+2*A41					[284]
$C_{12}H_8N_2$		benzo[c]cinnoline					
	432.2	20.92	0	48.4	51.2	20.92	22.1
		8*A10+4*A12+2*A41					[285]
$C_{12}H_8N_2O_5$		4,4′-dinitrodiphenyl ether					
	418.2	10.29	0	24.61	69.6	10.29	29.1
		8*A10+4*A12+2*A50+A32					[217]
$C_{12}H_8O$		dibenzofuran					
	355.7	18.6	0	52.29	52.3	18.6	18.6
		A14+2*A15+A112+2*A19+8*A10+2*A19					[286]
$C_{12}H_8OS$		phenoxathiin					
	328.8	20.27	0	61.63	58.9	20.27	19.4
		3*A15+A14+4*A19+8*A10+A131+A112					[12]
$C_{12}H_8OS_2$		diphenylene-2,2′-disulfide S-oxide					
	407	17.99	0	44.2	56.6	17.99	23.1
		8*A10+A14+3*A15+4*A19+A133					[216]
$C_{12}H_8O_2$		dibenzodioxin					
	395.7	23.2	0	58.63	57.2	23.2	22.6
		A14+3*A15+4*A19+8*A10+2*A112					[20]
$C_{12}H_8S$		dibenzothiophene					
	371	21.58	0	58.17	53.9	21.58	20.0
		A14+2*A15+2*A19+2*A19+A131+8*A10					[216]
$C_{12}H_8S_2$		dibenzo[c,e][1,2]dithiin					
	386.2	19.3	0	49.97	48.3	19.3	18.7
		A14+3*A15+2*A19+2*A19+8*A10+A132					[44]
$C_{12}H_8S_2$		thianthrene					
	429.6	27.55	0	64.13	60.5	27.55	26.0
		3*A15+A14+8*A10+4*A19+2*A131					[12]
$C_{12}H_9Cl$		2-chlorobiphenyl					
	304.9	14.54	0	47.7	55.1	14.54	16.8
		3*A12+9*A10+A22					[215]
$C_{12}H_9Cl$		4-chlorobiphenyl					
	348.6	13.32	0	38.2	55.1	13.32	19.2
		2*A12+9*A10+A22+A12					[215]
$C_{12}H_9ClN_2$		4-chloroazobenzene					
	361.2	27.2	0	75.3	57.0	27.2	20.6
		9*A10+3*A12+2*A42+A22*B22					[13]
$C_{12}H_8Cl_2O_3S$		4-chlorophenylbenzenesulfonate					
	332.2	21.44	0	64.53	68.4	21.44	22.7
		9*A10+3*A12+A22*B22+A89					[221]
$C_{12}H_9Cl_3Si$		*o*-trichlorosilylbiphenyl					
	289.5	0.06	0.2				
	339.2	20.72	61.09	61.28	63.6	20.78	21.6
		9*A10+2*A12+A11+3*A22*D22+A109					[216][62]
$C_{12}H_9Cl_3Si$		*p*-trichlorosilylbiphenyl					
	372.9	18.57	0	49.8	63.6	18.57	23.7
		9*A10+2*A12+A11+3*A22*D22+A109					[216,62]
$C_{12}H_9Cl_3Si$		4-trichlorosilylbiphenyl					
	372.9	18.57	0	49.8	65.8	18.57	24.5
		9*A10+3*A12+A109+3*A22*D22					[216]
$C_{12}H_9N$		carbazole					
	521	27.2	0	52.2	53.2	27.2	27.5
		A14+2*A15+2*A19+2*A19+8*A10+A121					[216]
$C_{12}H_9NS$		10H-phenothiazine					
	458.2	26.92	0	58.75	59.8	26.92	27.4
		A14+3*A15+4*A19+8*A10+A121+A131					[215]
$C_{12}H_{10}$		acenaphthene					
	366.6	21.46	0	58.55	41.09	21.46	15.0
		6*A10+A14+2*A15+3*A19+A12					[216]
$C_{12}H_{10}$		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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		10*A10+2*A12					[216]
$C_{12}H_{10}N_2$		*trans*-azobenzene					
	341.1	22.53	0	66.06	55.7	22.53	19.0
		10*A10+2*A12+2*A42					[216]
$C_{12}H_{10}N_2O$		azoxybenzene					
	309.2	17.93	0	57.99	64.3	17.93	19.9
		10*A10+2*A12+A54+A42					[215]
$C_{12}H_{10}N_2O$		4-hydroxyazobenzene					
	425.2	32.99	0	77.59	61.0	32.99	26.0
		9*A10+3*A12+2*A42+A31					[13]
$C_{12}H_{10}N_4O_2$		4-(4-nitrophenylazo)aniline					
	488.2	31.88	0	65.3	65.0	31.88	31.7
		8*A10+4*A12+2*A42+A50+A45					[13]
$C_{12}H_{10}O$		*o*-hydroxybiphenyl					
	330.6	16.21	0	48.12	64.6	16.21	21.3
		9*A10+A31+3*A12					[63]
$C_{12}H_{10}O$		diphenyl ether					
	300	17.21	0	57.32	63.9	17.21	19.2
		10*A10+2*A12+A32					[216]
$C_{12}H_{10}O_2$		1-naphthaleneacetic acid					
	405.3	22.26	0	54.92	47.8	22.26	19.4
		7*A10+2*A12+A11+A2+A36					[215]
$C_{12}H_{10}O_2$		2-carbomethoxynaphthalene					
	350.2	27.1	0	77.4	54.7	27.1	19.2
		7*A10+A1+A38+3*A12					[247]
$C_{12}H_{10}O_2$		1-acetoxynaphthalene					
	319.2	20.21	0	63.31	54.7	20.21	17.5
		7*A10+3*A12+A1+A38					[118]
$C_{12}H_{10}O_2$		2-acetoxynaphthalene					
	342.2	20.05	0	58.59	54.7	20.05	18.7
		7*A10+3*A12+A1+A38					[118]
$C_{12}H_{11}Cl_2NO$		3,5-dichloro-N-(1,1-dimethyl-2-propynyl)benzamide					
	428.4	28.68	0	66.94	58.1	28.68	24.9
		3*A12+3*A10+A60+2*A22*C22+2*A1+A4*B4+A8+A9					[221]
$C_{12}H_{11}N$		diphenylamine					
	326.2	17.86	0	54.75	53.9	17.86	17.6
		10*A10+2*A12+A44					[215]
$C_{12}H_{11}N$		2-aminobiphenyl					
	322.3	13.99	0	43.4	65.7	13.99	21.2
		9*A10+3*A12+A45					[205]
$C_{12}H_{11}NO$		1-naphthaleneacetamide					
	455.5	32.82	0	72.05	62.4	32.82	28.4
		7*A10+2*A12+A11+A2+A61					[221]
$C_{12}H_{11}NO_2$		1-naphthyl methylcarbamate					
	416.3	24.51	0	58.88	57.6	24.51	24.0
		7*A10+3*A12+A1+A69					[221]
$C_{12}H_{11}N_3$		*p*-phenylazoaniline					
	398.2	21.7	0	54.5	62.1	21.7	24.7
		9*A10+3*A12+2*A42+A45					[13]
$C_{12}H_{12}$		1,8-dimethylnaphthalene					
	336.3	15.77	0	46.9	45.5	15.77	15.3
		2*A1+2*A11+6*A10+2*A12					[215]
$C_{12}H_{12}$		2,6-dimethylnaphthalene					
	383.3	25.06	0	65.39	45.5	25.06	17.4
		2*A1+2*A11+6*A10+2*A12					[215]
$C_{12}H_{12}$		2,7-dimethylnaphthalene					
	368.8	23.35	0	63.3	45.5	23.35	16.8
		2*A1+2*A11+6*A10+2*A12					[215]
$C_{12}H_{12}$		1,4-dimethylnaphthalene					
	279.9	10.6	0	37.87	45.5	10.6	12.7
		2*A1+2*A11+2*A12+6*A10					[215]
$C_{12}H_{12}$		2,3-dimethylnaphthalene					
	378	15.9	0	42.06	45.5	15.9	17.2
		2*A1+2*A11+2*A12+6*A10					[215]
$C_{12}H_{12}Ge$		diphenylgermane					
	240.2	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		10*A10+2*A12+A103					[133]
$C_{12}H_{12}N_2$		hydrazobenzene					
	407.2	17.65	0	43.34	48.6	17.65	19.8
		10*A10+2*A12+2*A44					[215]
$C_{12}H_{12}N_2O$		4′4′-diaminodiphenyl ether					
	465.4	7.74	0	16.63	76.8	7.74	35.8
		8*A10+4*A12+2*A45+A32					[216]
$C_{12}H_{12}O_4$		1,4-dimethylcubane dicarboxylate					
	437.8	41	0	93.65	34.0	41	14.9
		5*A14−7*A15+6*A16+2*A17+2*A1+2*A38					[340]
$C_{12}H_{12}O_6$		1,2,3-tricarbomethoxybenzene					
	375.7	32.7	0	87.04	75.6	32.7	28.4
		3*A1+3*A38+3*A12+3*A10					[217]
$C_{12}H_{13}ClF_3N_3O_4$		N-(2-chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzeneamine					
	318.4	23.08	0	72.49	75.5	23.08	24.0
		2*A10+3*A112+A11+4*A2+A1+A4*B4+3*A25+2*A50+A43+A22*G22					[221]
$C_{12}H_{13}NO_2$		4-methyl-7-dimethylaminocoumarin					
	416.1	23.92	0	57.47	53.0	23.92	22.0
		A14+3*A15+A115+2*A19+A19+A18*B18+3*A1+3*A10+A12+A43					[216]
$C_{12}H_{13}NO_4S$		2,3-dihydro-6-methyl-5-phenylcarbamoyl-1,4-oxathiin-4,4-dioxide					
	401.5	26.66	0	66.39	59.4	26.66	23.8
		A14+3*A15+A112+A1+2*A19+A134+A60+5*A10+A12					[221]
$C_{12}H_{14}N_2O_5$		2-cyclohexyl-4,6-dinitrophenol					
	378.7	28.03	0	74.02	68.3	28.03	25.9
		A14+3*A15+A16+2*A10+A11+3*A12+A31+2*A50					[232]
$C_{12}H_{14}N_4O$		3,3′,4,4′-tetraaminodiphenyl ether					
	402.6	25.3	0	62.84	89.8	25.3	36.2
		4*A45+6*A12+6*A10+A32					[227]
$C_{12}H_{14}O_4$		diethyl *o*-phthalate					
	269.9	17.99	0	66.66	79.5	17.99	21.5
		4*A10+2*A38+2*A12+2*A2+2*A1					[216]
$C_{12}H_{14}O_4$		diethyl terephthalate					
	317.2	24.69	0	77.82	79.5	24.69	25.2
		4*A10+2*A38+2*A12+2*A2+2*A1					[216]
$C_{12}H_{15}ClNO_4S_2$		S-6-chloro-2,3-dihydro-2-oxobenzoxazol-3-ylmethyl O,O-diethyl phosphorodithioate					
	320.0	30.03	0	93.86	89.0	30.03	28.5
		A14+2*A15+A126+2*A19+3*A10+A12+A22*C22+3*A2+2*A1+A80					[221]
$C_{12}H_{15}NO_2$		phenylaminoethyl methacrylate					
	297.5	25.47	0	85.6	70.4	25.47	21.0
		5*A10+A12+A44+2*A2+A1+A5+A7+A38					[216]
$C_{12}H_{15}NO_3$		2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate					
	426.24	30.33	0	71.17	61.0	30.33	26.0
		A14+2*A15+A17+2*A19+A112+3*A10+A12+3*A1+A69					[221]
$C_{12}H_{15}N_2O_3PS$		O,O-diethyl O-quinoxalin-2-yl phosphothioate					
	304.1	25.4	0	83.5	87.0	25.4	26.5
		5*A10+3*A12+2*A41+2*A1+2*A2+A79					[221]
$C_{12}H_{15}N_5O_4$		9-[(2-acetoxyethoxy)methyl]-2-acetylamino-9H-purine					
	407.2	42.33	0	104.0	86.5	42.33	35.2
		A14+2*A15+2*A19+A18*B18+A118+A119+					[203]
		2*A41+A10+A12+A60+2*A1+3*A2+A38+A32					
$C_{12}H_{15}N_5O_5$		9-[(2-acetoxyethoxy)methyl]-2-acetylamino-1,9-dihydro-6H-purin-6-one					
	477.2	47.37	0	99.27	92.8	47.37	44.3
		2*A14+3*A15+3*A19+A18*B18+2*A118+A119+A124+A60+2*A1+3*A2+A38+A32					[203]
$C_{12}H_{16}$		cyclohexylbenzene					
	280.5	15.3	0	54.55	57.2	15.3	16.1
		A14+3*A15+5*A10+A11+A16					[216]
$C_{12}H_{16}Cl_2N_2O$		N-butyl-N′-(3,4-dichlorophenyl)-N-methylurea					
	374.3	27.23	0	72.75	86.2	27.23	32.3
		2*A1+3*A2+3*A10+3*A12+2*A22*C22+A64*B64					[221]
$C_{12}H_{16}NO_2$		5-isopropyl-*m*-tolyl methylcarbamate					
	361.3	23.04	0	63.77	60.1	23.04	21.7
		4*A1+A3+2*A11+A12+3*A10+A69					[221]
$C_{12}H_{16}N_2O_2$		4-dimethylamino-3,5-xylyl methylcarbamate					
	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_{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)
$C_{12}H_{16}N_3O_6S$		4-methylsulphonyl-2,6-dinitro-N,N-dipropylaniline					
	424.3	28.05	0	66.1	79.7	28.05	33.8
		3*A1+4*A2+4*A12+2*A10+A43+2*A50+A88					[221]
$C_{12}H_{16}N_3O_3PS_2$		S-(3,4-dihydro-4-oxobenzo[d]-[1,2,3]-triazin-3-ylmethyl) O,O-diethyl phoshorodithioate					
	322.2	25.22	0	78.26	75.9	25.22	24.4
		A14+3*A15+2*A118+2*A19+4*A10+A125+3*A2+2*A1+A80					[221]
$C_{12}H_{17}NO_2$		pentyl 4-aminobenzoate					
	325.1	23.93	0	73.61	89.9	23.93	29.2
		4*A10+2*A12+A1+4*A2+A45+A38					[215]
$C_{12}H_{18}$		hexamethylbenzene					
	383.7	1.76	4.58				
	438.7	20.63	47.02	51.6	47.9	22.38	21.0
		6*A1+6*A11					[216]
$C_{12}H_{18}N_2O$		N,N-dimethyl-N′-[4-(1-methylethyl)phenyl]urea					
	430.5	33.87	0	78.68	66.7	33.87	28.7
		4*A1+A3+4*A10+A11+A12+A64					[215]
$C_{12}H_{18}N_2O_2$		3,5-dimethyl-4-(dimethylamino)phenyl methylcarbamate					
	361.7	18.37	0	50.79	56.9	18.37	20.6
		5*A1+2*A10+2*A11+2*A12+A43+A69					[215]
$C_{12}H_{18}N_4O_2$		8-pentyltheophylline					
	498.4	35.1	0	70.43	81.6	35.1	40.7
		2*A14+3*A15+2*A125+A118+A121+3*A1+3*A19+4*A2					[215]
$C_{12}H_{18}N_4O_6S$		4-(N,N-dipropylamino)-3,5-dinitrobenzenesulphonamide					
	414.8	38.48	0	92.78	90.2	38.48	37.4
		2*A1+4*A2+2*A10+4*A12+2*A50+A43+A96					[221]
$C_{12}H_{18}O_2$		4-hexylresorcinol					
	341.5	19.04	0	55.75	91.5	19.04	31.2
		3*A10+A11+2*A12+A1+5*A2+2*A31					[215]
$C_{12}H_{19}ClNO_3$		N-methyl O-methyl O-2-chloro-4-*tert*-butylphenyl phosphoramidate					
	332.0	21.98	0	66.19	66.2	21.98	22.0
		5*A1+A4+2*A12+A11+3*A10+A78+A22*B22					[221]
$C_{12}H_{20}$		1,3-dimethyladamantane					
	221	7.36	33.3				
	245	0.92	3.76	37.06	40.4	8.28	9.9
		3*A14+A15+2*A16+2*A17+2*A1					[146]
$C_{12}H_{20}N_4O_2$		3-cyclohexyl-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione					
	389.6	20.36	0	52.26	49.5	20.36	19.3
		2*A14+6*A15+2*A125+A16+3*A1+3*A43+A19+A118					[221]
$C_{12}H_{20}O_2$		1,7-cyclododecanedione					
	405.2	15.77	0	38.93	64.0	15.77	25.9
		A14+9*A15+2*A114					[114]
$C_{12}H_{20}O_3$		3,3,6,6-tetramethyloctanedioic anhydride					
	344.2	18.83	0	54.7	59.1	18.83	20.33
		A14+6*A15+4*A1+2*A17+A117					[109]
$C_{12}H_{20}O_4$		1,5-cyclooctanedione bis ethylene ketal					
	296.2	18.03	0	60.88	61.8	18.03	18.3
		3*A14+7*A15+4*A112+2*A17					[114]
$C_{12}H_{22}$		bicyclohexyl					
	256.1	1.54	6.01				
	267.5	0.74	2.77				
	273.5	7.08	25.89				
	277.2	6.78	24.46	59.13	59.5	15.4	16.5
		2*A14+6*A15+2*A16					[216]
$C_{12}H_{22}N_2O_2$		1,8-diaza-2,9-dioxocyclotetradecane					
	517.4	13.6	26.29				
	617.8	49.3	79.8	106.1	79.5	62.9	49.1
		A14+11*A15+2*A124					[248]
$C_{12}H_{22}N_6$		1-(piperidinyl)-3,5-(dimethylamino)-*s*-triazine					
	361.5	23.22	0	64.23	61.3	23.22	22.2
		A14+3*A15+A119+4*A1+2*A43+3*A12+3*A41					[215]
$C_{12}H_{22}O_2$		octyl methacrylate					
	230.3	24.9	0	104.6	114.8	24.9	26.4
		2*A1+A7+A5+A38+7*A2*B2					[227]
$C_{12}H_{22}O_2$		nonyl acrylate					
	236.5	23.36	0	98.78	121.2	23.36	28.7
		A1+A6*B6+A5+A38+8*A2*B2					[216]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{12}H_{22}O_4$		dodecanedioic acid					
	402.5	50.57	0	125.64	125.5	50.6	50.53
		10*A2*B2+2*A36*B36					[216]
$C_{12}H_{22}O_4$		di-*n*-butyl succinate					
	244.1	29.21	0	119.65	107.6	29.21	26.3
		2*A1+8*A2+2*A38					[216]
$C_{12}H_{23}N_7$		1-(4′-methylpiperizinyl)-3,5-bis(dimethylamino)-*s*-triazine					
	354.2	20.42	0	57.65	59.6	20.42	21.1
		5*A1+2*A43+3*A41+3*A12+A14+3*A15+2*A119					[242]
$C_{12}H_{24}$		cyclododecane					
	199	0.6	3.02				
	333.8	14.8	44.34	47.35	66.7	15.4	22.3
		A14+9*A15					[181]
$C_{12}H_{24}$		1-dodecene					
	212.9	4.55	21.38				
	237.9	19.87	83.54	104.92	124.1	24.43	29.5
		A1+9*A2*B2+A5+A6					[216]
$C_{12}H_{24}N_2O_2$		N,N′-di-*n*-propyladipamide					
	452	36.11	0	79.91	95.1	36.11	43.0
		4*A2+2*A1+2*A60+4*A2					[282]
$C_{12}H_{24}O_2$		dodecanoic acid					
	316.9	36.65	0	115.7	124.3	36.7	39.4
		10*A2*B2+A1+A36					[216]
$C_{12}H_{24}O_4$		2,2,8,8-tetramethyl-1,3,7,9-tetraoxycyclododecane					
	383.0	23.4	0	61.1	72.7	23.4	27.9
		A14+9*A15+4*A112+4*A1+2*A17					[47]
$C_{12}H_{24}O_4$		1,3,9,11-tetraoxacyclohexadecane					
	332.0	35.56	0	107.1	86.4	35.56	28.7
		A14+13*A15+4*A112					[117]
$C_{12}H_{24}O_6$		1,4,7,10,13,16-hexaoxacyclooctadecane					
	312.2	34	0	108.9	96.2	34	30.0
		A14+15*A15+6*A112					[120]
$C_{12}H_{25}NO_3$		N-decylglycine					
	387.6	42.2	0	108.9	119.5	42.2	46.3
		A19+9*A2*B2+A44+A36*B36+A2					[249]
$C_{26}H_{26}$		dodecane					
	263.6	36.82	0	139.75	128.5	36.82	33.9
		2*A1+10*A2*B2					[216]
$C_{12}H_{26}O$		1-dodecanol					
	300.2	40.17	0	133.76	122.0	40.17	36.6
		11*A2*B2+A1+A30					[217]
$C_{12}H_{26}O_3$		3-(*n*-nonyloxy)-1,2-propanediol					
	297.2	29.5	0	99.26	135.5	29.5	40.3
		A1+8*A2*B2+A32+2*A30*C30+A3*B3+2*A2					[217]
$C_{12}H_{27}ClSn$		tri-*n*-butyltin chloride					
	260.2	11.43	0	43.93	108.9	11.43	28.3
		3*A1+9*A2+A22*B22+A110					[130]
$C_{12}H_{30}O_3Si_3$		1,1,3,3,5,5-hexaethylcyclotrisiloxane					
	160	0.46	2.89				
	242.3	11.82	48.8				
	280.2	11.42	40.77	92.46	92.4	23.71	25.9
		6*A1+6*A2+3*A112+3*A139+A14+3*A15					[227]
$C_{12}H_{36}Si_6$		cyclododecamethylhexasilane					
	352.4	16.7	47.39				
	528.8	4.2	7.94	55.33	47.3	20.9	25.0
		A14+3*A15+6*A139+12*A1					[175]
$C_{13}H_5N_3O_7$		2,4,7-trinitrofluoren-9-one					
	430.2	2.9	6.74				
	449.2	23.5	52.32	59.06	50.8	26.4	22.8
		A14+2*A15+2*A19+2*A19+4*A10+3*A12+3*A50+A114					[198]
$C_{13}H_6Cl_6O_2$		2,2′-methylenebis(3,4,6-trichlorophenol)					
	437.6	33.26	0	76.01	80.6	33.26	35.3
		2*A10+8*A12+2*A11+6*A22*G22+A2+2*A31					[215]
$C_{13}H_7F_3N_2O_5$		2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene					
	364.6	18.44	0	50.58	69.4	18.44	25.3
		7*A10+4*A12+A11+A4*B4+3*A25+2*A50+A32					[215]
$C_{13}H_8Br_3NO_2$		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_{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)
	497.7	28.67	0	57.6	74.0	28.67	36.8
		6*A10+6*A12+3*A21+A31+A60					[221]
$C_{13}H_8Cl_2O$		*p, p′*-dichlorobenzophenone					
	420	30.12	0	71.71	66.3	30.12	27.9
		2*A22*C22+A35+8*A10+4*A12					[215]
$C_{13}H_8O$		xanthene					
	373.7	19.2	0	51.38	56.0	19.2	20.9
		A14+3*A15+2*A19+8*A10+A112+2*A19					[215]
$C_{13}H_8O$		9-fluorenone					
	356.4	18.12	0	50.84	49.7	18.12	17.7
		8*A10+A14+2*A15+2*A19+A114+2*A19					[215]
$C_{13}H_8OS$		thioxanthone					
	487.9	35.5	0	72.76	56.3	35.5	27.5
		A14+3*A15+4*A19+A114+A131+8*A10					[160]
$C_{13}H_8O_2$		xanthone					
	449.7	26.12	0	58.08	54.6	26.12	24.6
		A14+3*A15+4*A19+A112+A114+8*A10					[216]
$C_{13}H_9Cl_3N_2O$		benzoic acid, 2,4,6-trichlorophenyl hydrazide					
	439.7	32.71	0	74.4	59.2	32.71	26.0
		7*A10+5*A12+3*A22*D22+A60+A44					[221]
$C_{13}H_9F_3N_2O_2$		2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid					
	476	38	0	79.83	72.8	38	34.6
		3*A25+A4*B4+7*A10+3*A12+A11+A44+A41+A36					[85]
$C_{13}H_9N$		acridine					
	383.2	18.58	0	48.48	47.7	18.58	18.3
		9*A10+2*A12+A41+2*A12					[284]
$C_{13}H_9N$		7,8-benzoquinoline					
	324.1	14.1	0	43.51	47.7	14.1	15.5
		9*A10+4*A12+A41					[216]
$C_{13}H_9N$		phenanthridine					
	354	0.02	0.06				
	379.7	22.83	60.12	60.18	47.7	22.85	18.1
		9*A10+4*A12+A41					[216]
$C_{13}H_9N_2$		2-phenylbenzimidazole					
	572.2	22.18	0	38.75	65.9	22.18	37.7
		9*A10+A118+A121+A14+2*A15+3*A19+A12					
$C_{13}H_{10}$		fluorene					
	387.9	19.58	0	50.48	51.0	19.58	19.8
		8*A10+A14+2*A15+4*A19					[216]
$C_{13}H_{10}BrCl_2O_2PS$		O-(4-bromo-2,5-dichlorophenyl)O-methyl phenylphosphonothioate					
	345.6	31.35	0	90.73	87.2	31.35	30.1
		7*A10+5*A12+A1+2*A22*D22+A21+A81					[221]
$C_{13}H_{10}Cl_2S$		*p*-chlorobenzyl *p*-chlorophenyl sulfide					
	343.8	32.22	0	93.71	68.9	32.22	23.7
		8*A10+3*A12+A11+2*A22*D22+A2+A84					[232]
$C_{13}H_{10}N_2$		diphenylcarbodiimide					
	287.4	18.55	0	64.54	52.9	18.55	15.2
		10*A10+2*A12+2*A42+A9					[227]
$C_{13}H_{10}N_2O$		1,3-diphenylurea					
	512	34.6	0	67.58	60.7	34.6	31.1
		10*A10+2*A12+A66					[215]
$C_{13}H_{10}O$		benzophenone					
	321.0	18.19	0	56.67	63.8	18.19	20.5
		10*A10+2*A12+A35					[80]
$C_{13}H_{10}S$		thioxanthene					
	401.8	26.1	0	64.96	57.6	26.1	23.2
		A14+3*A15+2*A19+2*A19+A131+8*A10					[215]
$C_{13}H_{11}N$		N-methylcarbazole					
	362.5	17.15	0	47.32	49.3	17.15	17.9
		A14+2*A15+2*A19+2*A19+A119+A1+8*A10					[216]
$C_{13}H_{11}NO$		benzanilide					
	436.5	29.61	0	67.84	60.6	29.61	26.5
		10*A10+2*A12+A60					[216]
$C_{13}H_{12}$		diphenylmethane					
	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{13}H_{12}NO$		1,3-diphenylurea					
	512.1	34.62	0	67.6	60.7	34.62	31.1
		10*A10+2*A12+A66					[216]
$C_{13}H_{12}O$		diphenylcarbinol					
	338.5	23	0	67.93	46.9	23	15.9
		10*A10+2*A11+A3*B3+A30					[216]
$C_{13}H_{13}BrS$		*2-n*-propyl-5-(4-bromophenyl)thiophene					
	360.4	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					
	305.6	16.76	0	54.84	85.6	16.76	26.2
		10*A10+A12+A11+A45+A2					[215]
$C_{13}H_{13}NO_2$		(*dl*) 2-(1-naphthoxy)propionamide					
	445	37.66	0	84.62	69.8	37.66	31.1
		7*A10+3*A12+A32+A3*B3+A1+A61					[273]
$C_{17}H_{13}NO_2$		(*d*) 2-(1-naphthoxy)propionamide					
	475	38.07	0	80.16	69.8	38.07	33.2
		7*A10+2*A12+A32+A3*B3+A1+A61+A12					[273]
$C_{13}H_{14}N_2$		*bis*-(4-aminophenyl)methane					
	363.7	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					
	162	0.08	0.5				
	323.8	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					
	381.1	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-5yl dimethylcarbamate					
	324.3	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-N,N-dipropyl-4-(trifluoromethyl)benzenamine					
	321.4	22.32	0	69.45	76.6	22.32	24.6
		2*A10+A11+3*A12+2*A50+A43+3*A25					[215]
		+A4*B4+2*A1+4*A2					
$C_{13}H_{16}F_3N_3O_4$		N-butyl-N-ethyl-2,6-dinitro-4-trifluoromethylaniline					
	338.5	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					
	273.6	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					
	245.6	11.28	0	45.93	47.6	11.28	11.7
		4*A1+2*A10+2*A11+A14+2*A15+A17+2*A19					[215]
$C_{13}H_{18}ClNO$		N-(4-chlorophenyl)-2,2-dimethylpentanamide					
	360.2	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]
$C_{13}H_{18}ClNO$		N-(3-chloro-4-methylphenyl)-2-methylpentanamide					
	353.2	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					
	584.3	42.31	0	72.41	64.0	42.31	37.4
		3*A14+6*A15+A16+A124+A125+2*A19					[221]
$C_{13}H_{18}O_5S$		*dl*-2-ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranyl methanesulfonate					
	344.1	26.25	0	76.28	68.3	26.25	23.5
		A14+2*A15+A19+A19+A17+A16+A122+4*A1+A2+3*A10+A12+A89					[221]
$C_{13}H_{19}NO_2$		hexyl N-phenylcarbamate					
	328	32.76	0	100	93.4	32.76	30.7
		5*A10+A12+A1+5*A2+A69					[102]
$C_{13}H_{19}N_3O_4$		N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine					
	327.5	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]
$C_{13}H_{21}N_2O$		N,N-dimethyl-N′-(octahydro-4,7-methano-1H-inden-5-yl)urea					
	436.5	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					
	228.2	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
		3*A14+A15+A16+3*A17+3*A1					[146]
$C_{13}H_{22}O_3$		3,3,7,7-tetramethylnonanedioic anhydride					
	396.2	20.5	0	51.75	62.8	20.5	24.9
		A14+7*A15+4*A1+2*A17+A117					[109]
$C_{13}H_{24}N_6$		1-(hexamethyleneimine)-3,5-bis(dimethylamino)-*s*-triazine					
	335.8	16.32	0	48.6	65.0	16.32	21.8
		A14*4*A15+A119+4*A1+2*A43+3*A12+3*A41					[242]
$C_{13}H_{24}O_2$		tridecanolactone					
	290.6	18.16	62.37				
	300.4	9.08	30.21	92.55	77.2	27.24	23.2
		A14+11*A15+A115					[216]
$C_{13}H_{24}O_4$		tridecanedioic acid					
	387.5	45.3	0	116.9	134.9	45.3	52.3
		11*A2*B2+2*A36*B36					[216]
$C_{13}H_{26}$		cyclotridecane					
	285.6	0.9	3.15				
	297.6	7.4	24.87	28.02	70.4	8.3	20.9
		A14+10*A15					[181]
$C_{13}H_{26}$		*n*-heptylcyclohexane					
	232.8	22.22	0	95.43	90.1	22.22	21.0
		A14+A16+A1+6*A2+3*A15					[216]
$C_{13}H_{26}O_2$		tridecanoic acid					
	307.1	8.72	28.41				
	315.0	33.74	107.11	135.52	133.6	42.47	42.1
		11*A2*B2+A1+A36					[216]
$C_{13}H_{26}O_2Si_3$		1,1,1,3,5,5,5-heptamethyl-3-phenyltrisiloxane					
	226.8	18.29	0	80.64	80.8	18.29	18.3
		7*A1+5*A10+A12+2*A32+3*A109					[216]
$C_{13}H_{27}NO_2$		3(*n*-nonylamino)-1,2-propanediol					
	343.2	53.2	0	155.01	125.5	53.2	43.1
		A1+8*A2*B2+A44+2*A30*C30+A3*B3+2*A2					[217]
$C_{13}H_{28}$		*n*-tridecane					
	255	7.66	30.04				
	267.8	28.49	106.27	136.31	137.8	36.15	36.9
		2*A1+11*A2*B2					[216]
$C_{13}H_{28}O$		tri-*tert*-butylmethanol					
	302	7.2	23.84				
	390	3.43	8.379	32.64	32.6	10.63	12.7
		9*A1+3*A4+A30+A4*B4					[216]
$C_{13}H_{28}O$		tridecanol					
	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
		A1+12*A2*B2+A30					[224]
$C_{13}H_{28}O_2S$		3(*n*-decylthio)-1,2-propanediol					
	291.9	17.3	59.27				
	311.9	17.3	55.47	114.73	142.3	34.6	44.4
		A1+9*A2*B2+A84+2*A30*C30+A3*B3+2*A2					[217]
$C_{13}H_{28}O_2$		3(*n*-decyloxy)-1,2-propanediol					
	311	38.9	0	125.08	144.9	38.9	45.1
		A1+9*A2*B2+A32+2*A30*C30+A3*B3+2*A2					[217]
$C_{13}H_{29}NO_2$		3(*n*-decylamino)-1,2-propanediol					
	346.6	54.8	0	158.11	134.9	54.8	46.8
		A1+9*A2*B2+A44+2*A30*C30+2*A2+A3*B3					[217]
$C_{14}H_7ClF_3NO_5$		5-[2-chloro-4-(trifluoromethyl)phenoxyl]-2-nitrobenzoic acid					
	436.6	37.67	0	86.27	83.0	37.67	36.2
		6*A10+A11+5*A12+A22*G22+A36*F36+A32+A50+A4*B4+3*A25					[221]
$C_{14}H_7ClO_2$		2-chloroanthraquinone					
	483.0	39	0	80.74	53.3	39	25.7
		A14+3*A15+4*A19+2*A114+A22*C22+A12+7*A10					[216]
$C_{14}H_8Cl_4$		1-chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl)benzene					
	349.8	23.84	0	68.17	72.7	23.84	25.4
		8*A10+4*A12+A7+A7+4*A22*D22					[221]
$C_{14}H_8Cl_4$		1,1-dichloro-2,2-bis(4-chlorophenyl)ethylene					
	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-dichloroethylidenebis(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-*m*-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_{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)
	306.5	12.8	0	41.77	54.7	12.8	16.8
		8*A10+A14+3*A15+4*A19					[216]
$C_{14}H_{12}$		*trans*-stilbene					
	398.2	27.4	0	68.81	69.7	27.4	27.8
		10*A10+2*A12+2*A6					[215]
$C_{14}H_{12}$		9-methylfluorene					
	319.2	16.32	0	51.13	53.9	16.32	17.2
		A14+2*A15+4*A19+A16+A1+8*A10					[252]
$C_{14}H_{12}F_3NO_4S_2$		1,1,1-trifluoro-*n*-[2-methyl-4-(phenylsulphonyl)phenyl]methane sulfonamide					
	418.4	31.79	0	75.97	68.7	31.79	36.0
		8*A10+A11+3*A12+A88+A95+A4*B4+3*A25+A1					[221]
$C_{14}H_{12}O_2$		diphenylacetic acid					
	420.4	31.25	0	74.34	58.7	31.25	24.7
		10*A10+2*A11+A3*B3+A36					[216]
$C_{14}H_{12}O_2$		benzyl benzoate					
	293.1	20.44	0	69.76	71.9	20.44	21.1
		10*A10+A11+A12+A2+A38					[221]
$C_{14}H_{12}O_4$		1,2-dicarbomethoxynaphthalene					
	358.2	27.6	0	77.05	65.1	27.6	23.3
		6*A10+4*A12+2*A1+2*A38					[217]
$C_{14}H_{12}O_4$		1,3-dicarbomethoxynaphthalene					
	378.7	30.5	0	80.54	65.1	30.5	24.64
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		1,4-dicarbomethoxynaphthalene					
	340.2	20.4	0	59.96	65.1	20.4	22.13
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		1,5-dicarbomethoxynaphthalene					
	392	26.4	0	67.35	65.1	26.4	25.5
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		1,6-dicarbomethoxynaphthalene					
	371.8	22.1	0	59.44	65.1	22.1	24.2
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		1,7-dicarbomethoxynaphthalene					
	363.2	20	0	55.07	65.1	20	23.6
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		2,3-dicarbomethoxynaphthalene					
	324.2	20.2	0	62.31	65.1	20.2	21.1
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{12}O_4$		2,7-dicarbomethoxynaphthalene					
	410.2	26.6	0	64.85	65.1	26.6	26.7
		6*A10+2*A12+2*A1+2*A38+2*A12					[217]
$C_{14}H_{14}$		1,2,3,4-tetrahydrophenanthrene					
	302.6	11.17	36.91				
	285	5.83	20.44				
	298	1.77	5.92	63.28	49.5	18.76	14.7
		A14+3*A15+2*A19+2*A12+6*A10					[31]
$C_{14}H_{14}$		phenyl-*o*-tolylmethane					
	279.8	19.24	0	68.78	62.6	19.24	17.5
		9*A10+3*A11+A1+A2					[216]
$C_{14}H_{14}$*		2,2′-dimethylbiphenyl					
	293.1	2.28	0	7.78	0	2.28	0
		Prediction not made					[216]
$C_{14}H_{14}$		1,2-diphenylethane					
	273.2	2.25	8.23				
	324.3	22.73	70.09	78.32	69.2	24.98	22.4
		10*A10+2*A11+2*A2					[216]
$C_{14}H_{14}$*		2-ethylbiphenyl					
	267.1	2.07	0	7.74	0	2.07	0
		Prediction not made					[216]
$C_{14}H_{14}$		1,2,3,4-tetrahydroanthracene					
	373.3	19.16	51.33				
	388	2.92	7.53	58.85	49.5	22.08	19.2
		A14+3*A15+2*A19+6*A10+2*A12					[216]
$C_{14}H_{14}Cl_2N_2O$		1-[2-(2,4-dichlorophenyl)-2-(propenyloxy)ethyl]-1H-imidazole					
	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					[221]
		+3*A10+2*A12+A11+2*A22*E22+A32					

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)
$C_{14}H_{14}NO_4PS$		O-ethyl O-(4-nitrophenyl)phenylphosphonothioate					
	308.2	25.05	0	81.28	74.2	25.05	22.9
		9*A10+3*A12+A1+A2+A81					[221]
$C_{14}H_{14}O_2$		(*dl*) 1,2-diphenyl-1,2-dihydroxyethane					
	393	31.38	0	79.85	71.9	31.38	28.2
		10*A10+2*A11+2*A3*B3+2*A30*B30					[273]
$C_{14}H_{14}O_2$		(*d*) 1,2-diphenyl-1,2-dihydroxyethane					
	420.5	34.31	0	81.59	71.9	34.31	30.2
		10*A10+2*A11+2*A3*B3+2*A30*B30					[273]
$C_{14}H_{14}O_3$		2-(6-methoxy-2-naphthyl)propionic acid					
	439.2	29.41	0	66.96	58.6	29.41	25.7
		6*A10+3*A12+A11+2*A1+A3*B3+A36*B36+A32					[33]
$C_{14}H_{14}O_3$		2-pivaloylindan-1,3-dione					
	381.5	25.99	0	68.12	62.9	25.99	24.0
		A14+2*A15+2*A19+2*A114+4*A10+3*A1+A4*B4+A35+A16					[215]
$C_{14}H_{15}N_3$		N,N-dimethyl-4-phenylazoaniline					
	389.2	23.08	0	59.3	53.7	23.08	20.9
		2*A1+A43+9*A10+3*A12+2*A42					[13]
$C_{14}H_{16}$		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
		7*A14−7*A15+12*A16					[127]
$C_{14}H_{16}ClN_3O_2$		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
		4*A10+2*A12+3*A1+A4*B4+A3*B3+A14+2*A15+2*A18*B18					[221]
		+2*A118+A22*F22+A119+A35+A32					
$C_{14}H_{16}F_3N_3O_4$		N-(cyclopropylmethyl)-2,6-dinitro-*n*-propyl-4-(trifluoromethyl)benzenamine					
	305.8	22.51	0	73.61	70.9	22.51	21.7
		3*A12+2*A10+A11+A4*B4+3*A25+2*A50+A43+A1+3*A2+A14+A16					[221]
$C_{14}H_{16}O_8$		1,2,3,4-tetracarbomethoxybenzene					
	404.7	40.4	0	99.79	85.9	40.4	34.8
		4*A1+4*A38+4*A12+2*A10					[217]
$C_{14}H_{16}O_8$		1,2,3,5-tetracarbomethoxybenzene					
	389.2	32.6	0	83.89	85.9	32.6	33.4
		4*A1+4*A38+4*A12+2*A10					[217]
$C_{14}H_{16}O_8$		1,2,4,5-tetracarbomethoxybenzene					
	416.7	35.7	0	85.4	85.9	35.7	35.8
		4*A1+4*A38+4*A12+2*A10					[217]
$C_{14}H_{17}ClNPO_4S_2$		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
		A14+2*A15+2*A19+4*A10+A128+4*A2+2*A1+A80					[221]
$C_{14}H_{17}NO_2$		4-methyl-7-diethylaminocoumarin					
	343.8	17.88	0	52.02	67.2	17.88	23.1
		A14+3*A15+2*A19+A19+A18*B18+A115+3*A10+A12+3*A1+2*A2+A43					[216]
$C_{14}H_{18}$		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
		2*A14+6*A15+4*A19+2*A10					[216]
$C_{14}H_{18}ClN_3O_2$		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
		A14+2*A15+2*A118+A119+2*A18*B18+2*A3*B3					[221]
		+A32+A22*F22+4*A10+2*A12+3*A1+A4+A30*F30					
$C_{14}H_{19}Cl_2NO_2$		4[*p*-[bis(2-chloroethyl)amino]benzene]butanoic acid					
	338.9	29.18	0	86.1	102.7	29.18	34.8
		3*A2+4*A2+4*A10+A11+A12+A36*D36+2*A22*D22+A4					[221]
$C_{14}H_{19}NO$		2-(dimethylamino)-1,2-diphenylethanone					
	334.2	22.38	0	66.97	64.7	22.38	21.6
		10*A10+A11+A12+A35*B35+A43+2*A1+A3*B3					[253]
$C_{14}H_{20}$		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
		5*A14−A15+8*A16					[216]
$C_{14}H_{20}$		1,8-cyclotetradecadiyne					
	370	22.6	0	61.06	55.3	22.6	20.4
		A14+11*A15+4*A20					[108]

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)
$C_{14}H_{20}O$		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-*a*]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)-*n*-(1-methylpropyl)-2,6-dinitrobenzeneamine					
	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]
$C_{14}H_{22}$		*n*-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-*tert*-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]
$C_{14}H_{24}$		*cis*-anti-*trans*-perhydrophenanthrene					
	313	11.16	0	35.64	59.7	11.16	18.7
		3*A14+5*A15+4*A16					[216]
$C_{14}H_{24}$		*cis*-syn-*trans*-perhydrophenanthrene					
	273	10.48	0	38.39	59.7	10.48	16.3
		3*A14+5*A15+4*A16					[216]
$C_{14}H_{24}$		*trans*-anti-*trans*-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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{14}H_{28}O_2$		tetradecanoic acid					
	327	45.1	0	137.92	142.9	45.1	46.7
		12*A2*B2+A1+A36					[216]
$C_{14}H_{28}O_4$		2,2,9,9-tetramethyl-1,3,8,10-tetraoxacyclotetradecane					
	409.4	30.5	0	74.5	80.1	30.5	32.8
		A14+11*A15+4*A112+4*A1+2*A17					[27]
$C_{14}H_{29}NO_3$		N-dodecylglycine					
	393.1	48.4	0	123.12	138.2	48.4	54.3
		A1+11*A2*B2+A2+A36*B36+A44					[249]
$C_{14}H_{29}NO_3$		N-octyl-L-leucine					
	357.1	7.6	21.28				
	398.1	29.3	73.6	94.88	110.0	36.9	43.8
		3*A1+7*A2*B2+A3+A3*B3+A36*B36+A44+A2					[249]
$C_{14}H_{29}NO_3$		N-octyl-DL-leucine					
	353.6	6.8	19.23				
	367.1	27.2	74.09	93.33	110.0	34.0	40.4
		3*A1+7*A2*B2+A3+A3*B3+A36*B36+A44+A2					[249]
$C_{14}H_{30}$		tetradecane					
	279	45.07	0	161.54	147.1	45.07	41.1
		2*A1+12*A2*B2					[216]
$C_{14}H_{30}O$		1-tetradecanol					
	311.2	47.01	151.04				
	310.8	25.1	80.75				
	306	1.8	5.86				
	311	23.81	76.57				
	311.6	22.01	70.71				
	311	49.37	158.75	158.75	140.6	49.37	43.7
		A1+13*A2*B2+A30					[224]
$C_{14}H_{30}O_2S$		3(*n*-undecylthio)-1,2-propanediol					
	280.2	2.5	8.92				
	289.1	4.9	16.95				
	295.2	4.6	15.58				
	317.4	18.3	57.66	99.11	151.6	30.3	48.1
		A1+10*A2*B2+A84+2*A30*C30+2*A2+A3*B3					[217]
$C_{14}H_{30}O_3$		3(*n*-undecyloxy)-1,2-propanediol					
	311.7	43.1	0	138.27	154.2	43.1	48.1
		A1+10*A2*B2+A32+2*A30*C30+2*A2+A3*B3					[217]
$C_{14}H_{31}NO_2$		3(*n*-undecylamino)-1,2-propanediol					
	348.8	58.2	0	166.86	144.2	58.2	50.3
		A1+10*A2*B2+A44+2*A30*C30+2*A2+A3*B3					[217]
$C_{15}H_{10}N_2O_2$		4,4′-diphenylmethane diisocyanate					
	313.6	27.3	0	87.06	78.5	27.3	24.6
		8*A10+2*A12+2*A11+2*A58+A2					[216, 104]
$C_{15}H_{11}ClF_3NO_4$		2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene					
	358.8	30.07	0	83.8	82.4	30.07	29.6
		6*A10+A11+5*A12+A1+A2+A4*B4+3*A25+A22*G22+A50+2*A32					[215]
$C_{15}H_{11}ClN_2O$		7-chloro-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one					
	216.7	34	0	156.9	69.7	34	15.1
		A14+4*A15+2*A121+A22*C22+A16+A19+A18+5*A10+A12					[216]
$C_{15}H_{12}$		4-methylphenanthrene					
	182	0.02	0.12				
	295	0.03	0.11				
	324.9	14.04	43.21	43.44	44.8	14.09	14.6
		A1+9*A10+4*A12+A11					[216]
$C_{15}H_{12}N_2O_3$		1,4-diamino-2-methoxyanthraquinone					
	515.2	35.29	0	68.5	72.4	32.29	37.3
		A14+3*A15+2*A114+4*A19+5*A10+2*A45+3*A12+A1+A32					[13]
$C_{15}H_{13}Cl_2NO_2$		1,1-(di-*p*-chlorophenyl)-2-nitropropane					
	354.3	21.39	0	60.38	66.8	21.39	23.7
		8*A10+2*A11+2*A12+A3+A3*B3+A1+2*A22*C22+A50					[221]
$C_{15}H_{14}O$		1,3-diphenylacetone					
	307.2	20.2	0	65.77	73.8	20.2	22.7
		10*A10+2*A11+2*A2+A35					[217]
$C_{15}H_{15}ClN_2O_2$		3-[4-[4-chlorophenoxy]phenyl]-1,1-dimethylurea					
	425.8	34.87	0	81.88	82.9	34.87	35.3
		8*A10+4*A12+2*A1+A22*C22+A32*C32+A64*B64					[215]
$C_{15}H_{15}N$		N-isopropylcarbazole					
	137.5	0.64	4.64				
	180	0.38	2.09				

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)
	395.2	17.73	44.86	51.6	57.2	18.75	22.6
		$A14+2*A15+2*A19+8*A10+2*A1+A3*B3+A119+2*A19$					[142]
$C_{15}H_{15}NO$		N-methyldiphenylacetamide					
	439.8	30.23	0	68.73	64.3	30.23	28.3
		$10*A10+2*A11+A3*B3+A1+A60$					[221]
$C_{15}H_{16}N_2O_2$		*a*-cyclopropyl-*a*-(4-methoxyphenyl)-5-pyrimidinemethanol					
	383.1	26.63	0	69.51	88.0	26.63	33.7
		$A14+7*A10+A1+A4*B4+2*A11+A12+2*A41+A30*D30+A32+A16$					[221]
$C_{15}H_{16}O$		*p*-*α*-cumylphenol					
	346.4	21.68	0	62.58	66.3	21.68	23.0
		$8*A10+3*A12+A11+2*A1+A3+A31$					[216]
$C_{15}H_{16}O_2$		4,4′dihydroxydiphenyl-2,2-propane					
	433	30.1	0	69.52	66.0	30.1	28.6
		$2*A1+A4+8*A10+2*A12+2*A11+2*A31$					[216]
$C_{15}H_{17}Br_2NO_2$		3,5-dibromo-4-hydroxybenzonitrile octanoyl ester					
	318.3	26.49	0	83.23	105.8	26.49	33.7
		$4*A12+2*A10+2*A21+A56+A38+A1+6*A2$					[221]
$C_{15}H_{18}Cl_2N_2O_3$		3-[2,4-dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-one					
	360.6	26.39	0	73.19	89.3	26.39	32.2
		$A14+2*A15+A19+A126+A118+5*A1$					[221]
		$+A3*B3+A4+4*A12+2*A10+2*A22*E22+A32$					
$C_{15}H_{18}N_2O_6$		2-sec-butyl-4,6-dinitrophenyl 3-methylcrotonate					
	341.3	18.89	0	55.37	80.2	18.89	27.4
		$4*A1+A2+A3+2*A10+3*A12+A11+2*A50+A38+A7+A6*B6$					[222]
$C_{15}H_{21}NO$		2-methyl-1-phenyl-2-(N-piperidinyl)-1-propanone					
	310.2	16.74	0	53.97	71.7	16.74	22.2
		$5*A10+A12+A4*B4+2*A1+A14+3*A15+A119+A35$					[254]
$C_{15}H_{21}NO_4$		methyl N-(2-methoxyacetyl)-N-(2,6-xylyl)-dl-alaninate					
	345.5	26.46	0	76.58	82.1	26.46	28.4
		$5*A1+A2+A3*B3+3*A10+2*A11+A12+A38+A32+A59$					[221]
$C_{15}H_{23}N_3O_2$		N-capryl-pyrazinamide					
	360.5	50.58	0	140.31	104.7	50.58	37.7
		$A1+6*A2+3*A10+A12+2*A41+A71$					[9]
$C_{15}H_{24}O$		2,6-di-*tert*-butyl-4-methylphenol					
	343.7	23.85	0	69.39	52.2	23.85	17.9
		$7*A1+2*A10+3*A11+A12+2*A4+A31$					[101]
$C_{15}H_{24}O_2$		2,6-di-*tert*-butyl-4-methoxyphenol					
	374.4	26.9	0	71.86	59.0	26.9	22.1
		$7*A1+2*A4+2*A11+2*A12+2*A10+A31+A32$					[114]
$C_{15}H_{28}O_2$		pentadecanolactone					
	283	27.3	96.47				
	308.5	6.99	22.65	119.12	84.6	34.29	26.1
		$A14+13*A15+A115$					[282]
$C_{15}H_{30}$		cyclopentadecane					
	210.1	8.5	40.46				
	336.6	8.5	25.25	65.71	77.8	17	26.2
		$A14+12*A15$					[181]
$C_{15}H_{30}$		*n*-decylcyclopentane					
	251.0	33.14	0	132.01	127.6	33.14	32.0
		$A14+A16+A1+9*A2*B2+2*A15$					[216]
$C_{15}H_{30}O$		2-pentadecanone					
	312.2	54.57	0	174.8	151.7	54.39	47.4
		$2*A1+A35+12*A2*B2$					[216]
$C_{15}H_{30}O_2$		pentadecanoic acid					
	318.7	8.12	25.48				
	325.7	41.52	127.49	152.97	152.3	49.64	49.6
		$13*A2*B2+A1+A36$					[216]
$C_{15}H_{30}O_2$		methyl myristate					
	291.6	50.21	0	172.17	154.8	50.21	45.1
		$2*A1+12*A2*B2+A38$					[217]
$C_{15}H_{31}NO_3$		N-decyl-L-valine					
	378.1	21.3	56.33				
	380.6	15.4	40.46	96.8	121.5	36.7	46.3
		$3*A1+A3+A3*B3+9*A2*B2+A44+A36*B36$					[249]
$C_{15}H_{31}NO_3$		N-decyl-DL-valine					
	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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
		3*A1+A3+A3*B3+9*A2*B2+A44+A36*B36					[249]
$C_{15}H_{31}NO_3$		N-dodecyl-L-alanine					
	356.1	37.6	0	105.59	139.0	37.6	49.5
		2*A1+11*A2*B2+A3*B3+A36*B36+A44					[249]
$C_{15}H_{32}$		*n*-pentadecane					
	270.9	9.17	33.85				
	283.1	34.6	122.17	156.02	156.5	43.77	44.3
		2*A1+13*A2*B2					[216]
$C_{15}H_{32}O$		1-pentadecanol					
	316	23.64	74.81				
	316.6	54.73	172.86	172.8	150.0	54.73	47.5
		A1+14*A2*B2+A30					[224]
$C_{15}H_{32}O_2S$		3(*n*-dodecylthio)-1,2-propanediol					
	299	18.1	60.54				
	325.5	20.3	62.37	122.9	160.9	38.4	52.4
		A1+11*A2*B2+A84+2*A30*C30+2*A2+A3*B3					[217]
$C_{15}H_{32}O_3$		3(*n*-dodecyloxy)-1,2-propanediol					
	323	51.4	0	159.13	163.5	51.4	52.8
		A1+11*A2*B2+A32+2*A30*C30+2*A2+A3*B3					[217]
$C_{15}H_{33}NO_2$		3(*n*-dodecylamino)-1,2-propanediol					
	351.9	62.1	0	176.47	153.5	62.1	54.0
		A1+11*A2*B2+A44+2*A30*C30+2*A2+A3*B3					[217]
$C_{16}F_{34}$		perfluorohexadecane					
	176.5	1.13	6.4				
	177.7	3.01	16.94				
	186.7	1.89	10.12				
	402.2	61.09	151.89	185.35	172.0	67.12	69.2
		16*A4*B4+6*A25+28*A26					[67]
$C_{16}H_{10}$		pyrene					
	120.8	0.29	2.39				
	423.8	17.36	40.97	43.36	43.8	17.65	18.6
		10*A10+4*A12+2*A13					[216]
$C_{16}H_{10}$		1,2-benzacenaphthene (fluoranthene)					
	383.4	18.74	0	48.89	36.5	18.74	14.0
		10*A10+5*A12+A13					[216]
$C_{16}H_{11}F_3O$		4-ethoxy-2′,3′,4′-trifluorodiphenylacetylene					
	356.8	32.2	0	90.25	73.4	32.2	26.2
		6*A10+6*A12+2*A9+A2+A1+3*A24+A32					[196]
$C_{16}H_{12}F_2$		4-ethyl-3′,4′-difluorodiphenylacetylene					
	301.2	16.6	0	55.11	64.8	16.6	19.5
		7*A10+A11+4*A12+2*A9+A2+A1+2*A24					[196]
$C_{16}H_{12}F_2O$		4-ethoxy-2′,4′-difluorodiphenylacetylene					
	343.4	27	0	78.63	71.64	27	24.6
		7*A10+5*A12+2*A9+A2+A1+2*A24+A32*C32					[196]
$C_{16}H_{13}FO$		4-ethoxy-4′-fluorodiphenylacetylene					
	354.4	22.8	0	64.33	69.9	22.8	24.8
		8*A10+4*A12+2*A9+A2+A1+A24*B24+A32					[196]
$C_{16}H_{12}Ge$		diphenyldiethynylgermane					
	320	20.1	0	62.81	48.3	20.1	15.5
		10*A10+2*A12+2*A8+2*A9+A102					[48]
$C_{16}H_{12}Si$		diphenyldiethynylsilane					
	316.2	19.67	0	62.21	52.2	19.67	16.5
		10*A10+2*A11+2*A8+2*A9+A109					[216]
$C_{16}H_{14}$		4,5,9,10-tetrahydropyrene					
	319.9	1.85	5.77				
	385.1	0.13	0.34				
	412.8	17.09	41.41	47.53	52.5	19.07	21.7
		2*A14+4*A15+6*A19+6*A10					[18]
$C_{16}H_{14}Cl_2O_3$		ethyl 2-hydroxy-2,2-bis-(4-chlorophenyl)acetate					
	310.4	23.48	0	75.64	90.0	23.48	27.9
		8*A10+2*A11+2*A12+A1+A2+A4*B4+2*A22*D22+A30*D30+A38					[215]
$C_{16}H_{14}Cl_2O_4$		methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate					
	314.4	27.08	0	86.13	89.3	27.08	28.1
		7*A10+5*A12+2*A1+A3*B3+A38+2*A32+2*A22*D22					[221]
$C_{16}H_{14}O_2$		1,2-dibenzoylethane					
	187	0.22	1.17				
	418.6	38.99	93.3	94.56	82.6	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_{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)
$C_{16}H_{14}O_6$		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]phenylcarbamate					
	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-*m*-tolylcarbamoyloxphenylcarbamate					
	423.8	39.62	0	93.49	83.6	39.62	35.4
	2*A1+3*A12+A11+8*A10+2*A69						[221]
$C_{16}H_{16}O_2$		(*d*) 2-(*p*-methoxyphenyl)propiophenone					

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	326	21.76	0	66.74	76.8	21.76	25.0
	9*A10+2*A12+A3*B3+2*A1+A32+A11+A35						[273]
$C_{16}H_{16}O_2$		(*dl*) 2-(*p*-methoxyphenyl)propiophenone					
	353	26.36	0	74.67	76.8	26.36	27.1
	9*A10+2*A12+A3*B3+2*A1+A32+A11+A35						[273]
$C_{16}H_{16}O_3$		2,2-dimethoxy-1,2-diphenylethanone					
	338.5	20.86	0	61.63	83.4	20.86	28.2
	10*A10+A11+A12+2*A1+2*A32*C32+A35+A4*B4						[28]
$C_{16}H_{17}NO$		N,N-dimethyl-2,2-diphenylacetamide					
	407.1	25.43	67.55	62.47	69.3	25.43	28.2
	2*A1+10*A10+2*A11+A3*B3+A59						[217]
$C_{16}H_{18}FN_3O_3$		1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic acid					
	500.2	32.97	0	65.91	82.5	32.97	41.3
	2*A14+6*A15+2*A119+A121+A114+3*A19 +A18*B18+2*A12+2*A10+A24+A36+A1+A2						[36]
$C_{16}H_{18}N_2O$*		4-*n*-butyl-4′-hydroxyazobenzene					
	351.6	5.25	0	14.93	0	5.25	0
	No prediction made						[131]
$C_{16}H_{18}N_4O_4$		N,N-(2-hydroxyethyl)-4-(4-nitrophenyl)azoaniline					
	484.2	32.43	0	66.97	92.1	32.43	44.6
	8*A10+4*A12+4*A2+2*A30*+E30*+2*A42+A43+A50						[13]
$C_{16}H_{19}BrO_2$		4-*trans*-(4-bromophenyl)cyclohexyl (E)-2-butenoate					
	388.2	28.4	0	73.16	79.6	28.4	30.9
	A14+3*A15+2*A16+4*A10+A11+A12+A21+A38 +A1+A6*B6+A6						[140]
$C_{16}H_{19}ClO_2$		4-*trans*-(4-chlorophenyl)cyclohexyl (E)-2-butenoate					
	386.2	30.2	0	78.2	78.2	30.2	30.2
	A14+3*A15+2*A16+4*A10+A11+A12+A38 +A1+A6*B6+A6+A22*B22						[140]
$C_{16}H_{19}FO_2$		4-*trans*-(4-fluorophenyl)cyclohexyl (E)-2-butenoate					
	354.2	25.1	0	70.86	78.6	25.1	27.9
	A14+3*A15+2*A16+4*A10+A11+A12+A38+A1+A6*B6+A6+A24						[140]
$C_{16}H_{19}N_3O_2$		N,N-(2-hydroxyethyl)-4-phenylazoaniline					
	407	29.96	0	73.61	89.3	29.96	36.3
	9*A10+3*A12+4*A2+2*A30*E30+2*A42+A43						[13]
$C_{16}H_{20}N_2$		tetracyclopropylsuccinonitrile					
	390	22.3	0	57.18	64.4	22.3	25.1
	4*A14+4*A16+2*A4*B4+2*A56						[216]
$C_{16}H_{20}O_6P_2S_3$		O,O,O′,O′-tetramethyl O,O′-thiodi-*p*-phenylene bis(phosphorothioate)					
	303.2	33.03	0	108.94	104.0	33.03	31.5
	8*A10+4*A12+A84+2*A79+4*A1						[221]
$C_{16}H_{22}NClO_3$		N-(chloroacetyl)-*n*-(2,6-diethylphenyl)glycine ethyl ester					
	318	23.84	0	74.97	96.6	23.84	30.7
	3*A1+5*A2+3*A10+2*A11+A12+A22*C22+A59+A38						[221]
$C_{16}H_{22}O_3Si_3$		1,1,3,3-tetramethyl-5,5-diphenylcyclotrisiloxane					
	338.0	22.19	0	65.66	69.3	22.19	23.4
	4*A1+A14+3*A15+3*A112+3*A139+10*A10+2*A11						[216]
$C_{16}H_{24}N_6$		1-(methylphenethylamino)-3,5-bis(dimethylamino)-*s*-triazine					
	334.2	20.04	0	59.96	73.2	20.04	24.5
	5*A1+2*A2+A11+5*A10+3*A41+3*A12+3*A43						[215]
$C_{16}H_{25}NO_2$		nonyl phenylcarbamate					
	327	28.07	0	85.77	132.4	28.07	43.3
	5*A10+A12+A1+8*A2*B2+A69						[102]
$C_{16}H_{28}O_2$		1,9-cylohexadecanedione					
	301.2	17.95	59.59				
	351.2	8.03	22.87	82.47	78.8	25.98	27.7
	A14+13*A15+2*A114						[114]
$C_{16}H_{28}O_4$		1,7-cyclododecanedione bis ethylene ketal					
	478.2	36.94	0	77.26	76.6	36.94	36.6
	3*A14+11*A15+2*A17+4*A112						[114]
$C_{16}H_{32}$		cyclohexadecane					
	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
	A14+13*A15						[112]
$C_{16}H_{32}$		*n*-decylcyclohexane					
	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_{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)
		9*A2*B2+A1+A14+3*A15+A16					[215]
$C_{16}H_{32}$		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(*n*-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(*n*-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(*n*-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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{17}H_{12}O$		4-ethynyl-1-[(4-ethynylphenyl)methoxy]benzene					
	371.2	21.2	0	57.11	63.4	21.2	23.5
		2*A9+2*A8+3*A12+A11+A2+A32+8*A10					[216]
$C_{17}H_{12}O_2$		4-benzoyl-1-naphthol					
	440.6	28.64	0	65	69.0	28.64	30.4
		11*A10+5*A12+A35+A31					[215]
$C_{17}H_{12}O_2$		1-benzoyl-2-naphthol					
	414.1	31.35	0	75.71	69.0	31.35	28.6
		11*A10+5*A12+A35+A31					[215]
$C_{17}H_{12}O_2$		2-benzoyl-1-naphthol					
	343.9	20.18	0	58.68	69.0	20.18	23.7
		11*A10+5*A12+A35+A31					[215]
$C_{17}H_{12}O_2$		1-naphthyl benzoate					
	329.2	16.98	0	51.58	66.7	16.98	22.0
		12*A10+4*A12+A38					[118]
$C_{17}H_{12}O_2$		2-naphthyl benzoate					
	381.2	26.23	0	68.81	66.7	26.23	25.4
		12*A10+4*A12+A38					[118]
$C_{17}H_{13}F_3O$		4-*n*-propoxy-2′,3′,4′-trifluorodiphenylacetylene					
	327.3	26.1	0	79.74	80.5	26.1	26.4
		6*A10+6*A12+3*A24+2*A2+A1+2*A9+A32					[196]
$C_{17}H_{14}F_2$		4-*n*-propyl-3′,4′-difluorodiphenylacetylene					
	311	20.2	0	64.95	72.0	20.2	22.4
		7*A10+A11+4*A12+2*A24+2*A2+A1+2*A9					[196]
$C_{17}H_{14}F_2O$		4-*n*-propoxy-2′,4′-difluorodiphenylacetylene					
	326.9	25.2	0	77.09	78.8	25.2	25.8
		7*A10+5*A12+2*A24+2*A2+A1+2*A9+A32					[196]
$C_{17}H_{14}N_2O_2$		2,2-bis-(4-cyanatophenyl)propane					
	355.8	26.69	0	75.02	71.7	26.69	25.51
		2*A1+A4+2*A11+2*A12+2*A58+8*A10					[216]
$C_{17}H_{14}O_5$		3-[1-(2-furanyl)-3-oxobutyl]-4-hydroxy-2H-1-benzopyran-2-one					
	391.8	33.88	0	86.49	87.5	33.88	34.3
		2*A14+5*A15+5*A19+2*A18+A18*B18+4*A10+A1					[221]
		+A2+A3+A35+A115+A112+A30*D30					
$C_{17}H_{15}F$		4-*n*-propyl-4′-fluorodiphenylacetylene					
	324	24.1	0	74.38	70.2	24.1	22.8
		8*A10+A11+3*A12+A24+2*A2+A1+2*A9					[196]
$C_{17}H_{15}FO$		4-*n*-propoxy-4′-fluorodiphenylacetylene					
	356.8	27.1	0	75.95	77.0	27.1	27.5
		8*A10+4*A12+A24+2*A2+A1+2*A9+A32					[196]
$C_{17}H_{16}Br_2O_3$		isopropyl 4,4′-dibromobenzilate					
	348.1	24.55	0	70.53	93.5	24.55	32.5
		8*A10+2*A11+2*A12+A30*D30+A38+2*A1+A3*B3+2*A21+A4*B4					[216]
$C_{17}H_{18}FN_3O_3$		1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-qiunolinecarboxylic acid					
	541.5	64.48	0	119.08	91.2	64.48	49.4
		3*A14+6*A15+3*A19+A18*B18+A114+2*A119					[36]
		+A121+2*A10+2*A12+A36*F36+A24					
$C_{17}H_{19}FNO_2$		4-*trans*-(3-fluoro-4-cyanophenyl)cyclohexyl (E)-but-2-enoate					
	393.2	21.1	0	53.66	81.5	21.1	32.0
		3*A10+2*A12+A11+A24+A56+A14+3*A15+2*A16+A38+A6+A6*B6+A1					[140]
$C_{17}H_{19}F_3O_3$		4-*trans*-(trifluoromethoxyphenyl)cyclohexyl (E)-but-2-enoate					
	340.2	21.6	0	63.49	83.6	21.6	28.4
		4*A10+A12+A11+3*A25+A14+3*A15+2*A16					[140]
		+A38+A6+A6*B6+A1+A32+A4*B4					
$C_{17}H_{21}NO_2$		N,N-diethyl-2-(1-naphthyloxy)propionamide					
	345.3	24.57	0	71.16	80.3	24.57	27.7
		3*A1+2*A2+B3*A3+7*A10+3*A12+A32+A59					[221]
$C_{17}H_{34}O$		9-heptadecanone					
	323.9	66.68	0	205.87	170.4	66.68	55.2
		2*A1+A35+A14*A2*B2					[21]
$C_{17}H_{34}O_2$		heptadecanoic acid					
	329.2	7.44	22.59				
	334.3	51.33	153.55	176.15	170.9	58.77	57.1
		15*A2*B2+A1+A36					[216]
$C_{17}H_{34}O_2$		methyl palmitate					
	307.2	68.16	0	221.84	173.5	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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
		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]
$C_{17}H_{36}$		*n*-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(*n*-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(*n*-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(*n*-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]
$C_{18}H_{14}$		*m*-terphenyl					
	360	22.59	0	62.76	73.9	22.59	26.6
		14*A10+4*A12					[256]
$C_{18}H_{14}$		*p*-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]
$C_{18}H_{14}$		*o*-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-*n*-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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{18}H_{15}OP$		triphenylphosphine oxide					
	431.9	24.22	0	56.08	56.1	24.22	24.2
		15*A10+3*A12+A73					[246]
$C_{18}H_{15}O_4P$		triphenyl phosphate					
	322.5	29.61	0	91.81	78.8	29.61	25.4
		15*A10+3*A12+A74					[215]
$C_{18}H_{15}P$		triphenylphosphine					
	354.4	19.69	0	55.56	68.0	19.69	24.1
		15*A10+3*A12+A72					[246]
$C_{18}H_{16}F_2$		4-*n*-butyl-3′,4′-difluorodiphenylacetylene					
	323.5	25.3	0	78.21	79.1	25.3	25.6
		7*A10+A11+4*A12+2*A24+3*A2+A1+2*A9					[196]
$C_{18}H_{16}O_3$		1,8-diphenyl-2,3,5-trioxabicyclo[4.3.0]non-7-ene					
	371.2	21.7	0	58.46	45.3	21.7	16.8
		10*A10+A11+A12+2*A14+3*A15+A19+A18+6*A16					[257]
		+A17+A112+A113					
$C_{18}H_{16}O_8$		1,2,3,4-tetracarbomethoxynaphthalene					
	423.7	35.9	0	84.47	85.8	35.9	36.3
		4*A1+4*A38+4*A10+6*A12					[217]
$C_{18}H_{16}O_8$		1,2,4,5-tetracarbomethoxynaphthalene					
	438.2	36.4	0	82.89	85.8	36.4	37.6
		4*A1+4*A38+4*A10+6*A12					[217]
$C_{18}H_{16}O_8$		1,2,5,6-tetracarbomethoxynaphthalene					
	470.2	42.1	0	89.37	85.8	42.1	40.3
		4*A1+4*A38+4*A10+6*A12					[217]
$C_{18}H_{16}O_8$		1,2,6,7-tetracarbomethoxynaphthalene					
	407.2	34.2	0	83.76	85.8	34.2	34.9
		4*A1+4*A38+4*A10+6*A12					[217]
$C_{18}H_{16}O_8$		2,3,6,7-tetracarbomethoxynaphthalene					
	458.2	42.2	0	91.88	85.8	42.2	39.3
		4*A1+4*A38+4*A10+6*A12					[217]
$C_{18}H_{16}O_8$		1,4,5,8-tetracarbomethoxynaphthalene					
	477.2	36.1	0	75.69	85.8	36.1	40.9
		4*A1+4*A38+4*A10+6*A12					[217]
$C_{18}H_{17}Cl_2NO_3$		ethyl N-benzoyl-*n*-(3,4-dichlorophenyl)-*dl*-alaninate					
	341.7	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]
$C_{18}H_{17}F$		4-*n*-butyl-4′-fluorodiphenylacetylene					
	329.9	18.5	0	56.08	77.4	18.5	25.5
		8*A10+A11+3*A12+A24+3*A2+A1+2*A9					[196]
$C_{18}H_{17}FO$		4-*n*-butoxy-4′-fluorodiphenylacetylene					
	346.7	25.4	0	73.26	84.2	25.4	29.4
		8*A10+4*A12+A24+3*A2+A1+2*A9+A32					[196]
$C_{18}H_{18}$		1-methyl-7-isopropylphenanthrene					
	369	18.03	0	48.87	46.6	18.03	17.2
		8*A10+3*A1+2*A11+A3+4*A12					[216]
$C_{18}H_{18}ClNS$		2-chloro-9-(3-dimethylaminopropylidene)-10-thioxanthene					
	370.3	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					[216]
		+2*A2+2*A1+A43					
$C_{18}H_{18}N_2O_2$		N,N′-(2-hydroxyethyl)-1,4-diaminoanthraquinone					
	521.2	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]
$C_{18}H_{18}O_2$		3-diphenylmethyl-2,4-pentanedione					
	387.2	27.02	0	69.78	73.3	27.02	28.4
		2*A1+A3*B3+2*A35+A3+10*A10+2*A11					[259]
$C_{18}H_{18}O_3$		butyl 9-hydroxy-9H-fluorene-9-carboxylate					
	343.9	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]
$C_{18}H_{20}Cl_2$		1,1′-(2,2-dichloroethylidene)bis(4-ethylbenzene)					
	331.6	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]
$C_{18}H_{20}O_2$		diethylstilbestrol					
	443.8	31.76	0	71.57	97.8	31.76	43.5
	441.8	28.8	0	65.1	97.8	28.8	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_{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)
$C_{18}H_{22}$		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-*trans*-(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-*tert*-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]
$C_{18}H_{30}O_4$		*p*-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]
$C_{18}H_{34}O_2$		*trans*-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]
$C_{18}H_{34}O_2$		*cis*-9-octadecenoic acid					
	286.5	39.6	0	138.24	172.1	39.6	49.3
		A1+14*A2*B2+2*A6+A36					[216]
$C_{18}H_{34}O_2$		*cis*-6-octadecenoic acid					
	303.7	47.5	0	156.43	172.1	47.5	52.3
		A1+14*A2*B2+2*A6+A36					[216]
$C_{18}H_{36}$		*n*-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-*n*-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_{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)
$C_{18}H_{36}O_4$		2,2,11,11-tetramethyl-1,3,10,12-tetraoxacyclooctadecane					
	373.0	35.1	0	94.1	94.9	35.1	35.4
		A14+15*A15+4*A112+2*A17+4*A1					[47]
$C_{18}H_{37}NO$		N-butyl tetradecanamide					
	336.1	45	0	133.89	170.0	45	57.1
		2*A1+3*A2+A60+12*A2*B2					[217]
$C_{18}H_{37}NO$		octadecanamide					
	377.2	59.91	0	158.84	194.8	59.91	73.5
		16*A2*B2+A1+A61					[217]
$C_{18}H_{37}NO_3$		N-hexadecylglycine					
	384.6	4.5	11.7				
	366.1	5.6	15.3				
	393.1	56.5	143.73	170.73	175.5	66.6	69.0
		15*A2*B2+A1+A44+A36*B36+A2					[249]
$C_{18}H_{37}NO_3$		N-dodecyl-L-luecine					
	383.1	33.5	0	87.44	147.3	33.5	56.4
		3*A1+11*A2*B2+A3+A3*+A36*B36+A44+A2					[249]
$C_{18}H_{37}NO_3$		N-dodecyl-DL-leucine					
	341.1	28.9	84.73				
	356.6	31	86.93	171.66	147.3	59.9	52.5
		3*A1+11*A2*B2+A3+A3*B3+A36*B36+A44+A2					[249]
$C_{18}H_{38}$		octadecane					
	301.3	61.5	0	204.6	184.5	61.5	55.6
		2*A1+16*A2*B2					[216]
$C_{18}H_{38}O$		octadecanol					
	334.2	70.08	0	209.7	178.0	70.08	59.5
		17*A2*B2+A1+A30					[220]
$C_{18}H_{48}Si_6$		1,2,3,4,5,6-hexamethyl-1,2,3,4,5,6-hexaethylcyclohexasilane					
	226.3	3.8	16.79				
	439.2	1.8	4.1	20.89	90.1	5.6	39.6
		A14+3*A15+6*A139+12*A1+6*A2					[175]
$C_{19}H_{13}F_3O$		4-ethoxy-4′-trifluoromethyldiphenyldiacetylene					
	424.9	32.73	0	77.03	62.9	32.73	26.7
		A1+A2+A11+3*A12+8*A10+4*A9+3*A25+A4*B4+A32					[195]
$C_{19}H_{14}F_2$		4-*n*-propyl-3′,4′difluorodiphenyldiacetylene					
	343.7	22.03	0	64.1	66.4	22.03	22.8
		A1+2*A2+A11+4*A12+7*A10+4*A9+2*A24					[195]
$C_{19}H_{15}Cl$		triphenylchloromethane					
	376.8	27.9	0	74.04	70.3	27.9	26.5
		15*A10+3*A11+A22+A4*B4					[216]
$C_{19}H_{16}$		triphenylmethane					
	365.3	21.97	0	60.13	66.0	21.97	24.1
		15*A10+A3+3*A11					[216]
$C_{19}H_{16}O_2$		2-fluorenyl-2-methyl-1,3-cyclopentanedione					
	395.2	24.6	0	62.25	57.4	24.6	22.7
		2*A14+4*A15+2*A114+A17+A1+A16+4*A19+8*A10					[259]
$C_{19}H_{17}F_3O$		4-*n*-pentoxy-2′,3′,4′-trifluorodiphenylacetylene					
	315.8	33.1	0	104.81	94.8	33.1	29.9
		6*A10+6*A12+3*A24+A32+4*A2+A1+2*A9					[196]
$C_{19}H_{18}F_2$		4-*n*-pentyl-3′,4′-difluorodiphenylacetylene					
	323.1	22.1	0	68.4	86.2	22.1	27.9
		7*A10+A11+4*A12+2*A24+4*A2+A1+2*A9					[196]
$C_{19}H_{18}O_2$		2-methyl-2-diphenylmethyl-1,3-cyclopentanedione					
	394.2	34.3	0	87.01	59.7	34.3	23.5
		A14+2*A15+2*A114+A17+A1+A3+2*A11+10*A10					[259]
$C_{19}H_{19}F$		4-*n*-pentyl-4′-fluorodiphenylacetylene					
	337.4	25.6	0	75.87	84.5	25.6	28.5
		8*A10+A11+3*A12+A24+4*A2+A1+2*A9					[196]
$C_{19}H_{19}FO$		4-*n*-pentoxy-4′-fluorodiphenylacetylene					
	330.9	27.2	0	82.2	91.3	27.2	30.2
		8*A10+4*A12+A24+4*A2+A1+2*A9+A32					[196]
$C_{19}H_{20}F_3N_3O_3$		2-[3-(trifluoromethyl)-phenyl]amino-3-pyridinecarboxylic acid β-morpholino ethyl ester					
	350	34.5	0	98.57	91.1	34.5	31.9
		A14+3*A15+A112+A119+2*A2+A38+7*A10+3*A12+A41+A44+A11+A4*B4+3*A25					[216]
$C_{19}H_{20}O_2$		3-methyl-3-diphenylmethyl-2,4-pentanedione					
	352.2	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		3*A1+A4*B4+2*A35+A3+10*A10+2*A11					[259]
$C_{19}H_{21}NO$		1,2-diphenyl-2-(N-piperidinyl)-1-ethanone					
	349.2	33.93	0	97.16	77.0	33.93	26.9
		10*A10+A11+A12+A35+A14+3*A15+A119+A3*B3					[253]
$C_{19}H_{23}NO$		*p*-*n*-hexyloxybenzylideneaniline					
	73.41	0.19	2.62				
	321.6	30.91	96.1	98.72	104.4	31.1	33.58
		9*A10+3*A12+A42+A32+5*A2+A1+A6*B6					[216]
$C_{19}H_{24}O$		2-*tert*-butyl-4-methyl-6-α-methylbenzylphenol					
	337.7	31.38	0	92.92	63.0	31.4	21.3
		5*A1+A4+4*A11+A12+7*A10+A31+A3					[101]
$C_{19}H_{26}O_2$		testosterone					
	428	29.45	0	68.81	60.2	29.45	25.9
		4*A14+5*A15+2*A17+4*A16+2*A1+A30*B30+A19+A18*B18+A114					[219]
$C_{19}H_{28}N_2$		4-(4-*n*-heptyl-1-piperidinyl)benzonitrile					
	326.2	29.01	0	88.95	103.2	29.1	33.7
		A14+3*A15+A119+A16+6*A2+A1+4*A10+2*A12+A56					[26]
$C_{19}H_{30}O_2$		5α-androstane-3-one-17β-ol					
	455.5	27.15	0	59.6	60.9	27.15	27.7
		4*A14+5*A15+2*A17+2*A1+5*A16+A30*B30+A114					[216]
$C_{19}H_{38}O$		2-nonadecanone					
	328	68.65	0	209.3	189.0	68.65	62.0
		A35+2*A1+16*A2*B2					[21]
$C_{19}H_{38}O$		10-nonadecanone					
	330	66.67	0	202.04	189.0	66.67	62.4
		A35+2*A1+16*A2*B2					[21]
$C_{19}H_{38}O_2$		nonadecanoic acid					
	338	9.76	28.87				
	341.2	57.62	168.87	195.93	189.6	67.38	64.7
		17*A2*B2+A1+A36					[216]
$C_{19}H_{38}O_2$		methyl octadecanoate					
	310.9	64.4	0	205.8	192.1	64.4	59.7
		2*A1+A38+16*A2*B2					[391]
$C_{19}H_{39}NO_3$		N-hexadecyl-L-alanine					
	374.1	65.3	0	174.55	176.3	65.3	66.0
		15*A2*B2+2*A1+A3*B3+A44+A36*B36					[249]
$C_{19}H_{39}NO_3$		N-tetradecyl-L-valine					
	334.6	14.9	44.53				
	365.1	20.6	56.42	100.95	158.8	35.5	58.0
		3*A1+A3+A3*B3+13*A2*B2+A44+A36*B36					[249]
$C_{19}H_{39}NO_3$		N-tetradecyl-DL-valine					
	370.1	68.1	0	184	158.8	68.1	58.8
		3*A1+A3+A3*B3+13*A2*B2+A44+A36*B36					[249]
$C_{19}H_{40}$		nonadecane					
	296.0	13.67	46.2				
	304	47.4	155.9	202.1	193.8	61.07	58.7
		2*A1+17*A2*B2					[216]
$C_{20}F_{42}$		perfluoroeicosane					
	149.5	0.67	4.48				
	202.9	11.25	55.45				
	437.9	80.33	183.44	243.37	211.6	92.25	92.6
		20*A4*B4+36*A26+6*A25					[67]
$C_{20}H_{12}$		perylene					
	551.0	31.88	0	57.87	43.7	31.88	24.1
		12*A10+6*A12+2*A13					[216, 217]
$C_{20}H_{12}$		1,2-benzopyrene					
	426.2	2.51	5.89				
	454.4	16.57	36.46	42.35	43.7	19.08	19.8
		12*A10+6*A12+2*A13					[215]
$C_{20}H_{12}$		3,4-benzopyrene					
	390.2	8.49	21.77				
	454.2	17.32	38.13	59.9	43.7	25.81	19.8
		12*A10+6*A12+2*A13					[215]
$C_{20}H_{14}$		triptycene					
	527.2	30.29	0	57.46	60.1	30.29	31.7
		2*A14+2*A15+2*A16+6*A19+12*A10					[216]
$C_{20}H_{14}$		β,β-binaphthyl					

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)
	461.2	38.9	0	84.35	58.9	38.9	27.2
		14*A10+6*A12					[216]
$C_{20}H_{14}O_4$		phenolphthalein					
	534	51.05	0	95.59	114.34	51.05	61.06
		A14+2*A15+A115+2*A19+A17+2*A31+12*A10					[216]
$C_{20}H_{15}F_3O$		4-propoxy-4′-trifluoromethyldiphenyldiacetylene					
	315.9	18.81	0	59.54	70.0	18.81	22.1
		A1+2*A2+A11+3*A12+8*A10+4*A9+3*A25+A4*B4+A32					[195]
$C_{20}H_{16}F_2$		4-*n*-butyl-3′,4′-diflurodiphenyldiacetylene					
	340.8	24.33	0	71.39	73.6	24.33	25.1
		A1+3*A2+A11+4*A12+7*A10+4*A9+2*A24					[195]
$C_{20}H_{18}O_2$		2-fluoroenyl-2-methyl-1,3-cyclohexanedione					
	448.2	35.7	0	79.65	61.1	35.7	27.4
		2*A14+5*A15+2*A114+A17+A1+A16+4*A19+8*A10					[259]
$C_{20}H_{18}O_2Sn$		(acetyloxy)triphenylstannane					
	397.6	41.92	0	105.44	89.8	41.92	35.7
		15*A10+3*A12+A1+A38+A110					[221]
$C_{20}H_{19}F_3O$		4-*n*-hexyloxy-2′,3′,4′-trifluorodiphenylacetylene					
	322	30.8	0	95.65	85.3	30.8	27.5
		A1+5*A2+6*A12+6*A10+2*A9+2*A24+A32					[196]
$C_{20}H_{20}F_2$		4-*n*-hexyl-3′,4′-difluorodiphenylacetylene					
	314.9	24.3	0	77.17	78.5	24.3	24.7
		A1+5*A2+A11+5*A12+6*A10+2*A9+2*A24					[196]
$C_{20}H_{20}F_2O$		4-*n*-hexyloxy-3′,4′-difluorodiphenylacetylene					
	323.6	33.1	0	102.29	85.3	33.1	27.6
		A1+5*A2+6*A12+6*A10+2*A9+2*A24+A32					[196]
$C_{20}H_{20}F_2O$		4-*n*-hexyloxy-2′,4′-difluorodiphenylacetylene					
	320.9	34.1	0	106.26	85.3	34.1	27.4
		A1+5*A2+6*A12+6*A10+2*A9+2*A24+A32					[196]
$C_{20}H_{20}O_2$		2-ethyl-2-diphenylmethyl-1,3-cyclopentanedione					
	382.2	28.2	0	73.78	66.8	28.2	25.5
		A14+2*A15+2*A114+A17+A1+A3+2*A11+10*A10+A2					[259]
$C_{20}H_{20}O_3$		4,4-dimethyl-1,8-diphenyl-2,3,5-trioxabicyclo[4.3.0]non-7-ene					
	369.2	22.1	0	59.86	45.9	22.1	16.9
		10*A10+A11+A12+2*A14+3*A15+A19+A18+A162+A17+A112+A113+2*A1					[257]
$C_{20}H_{22}O_2$		3-ethyl-3-diphenylmethyl-2,4-pentanedione					
	388.2	34.7	0	89.39	84.8	34.7	32.9
		3*A1+A4*B4+2*A35+A3+10*A10+2*A11+A2					[259]
$C_{20}H_{26}O_2$		19-nor-17α-ethylnyltestosterone					
	479	39.6	0	82.67	55.1	39.6	26.4
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114					[216]
		+A30*B30+A1+A8+A9					
$C_{20}H_{26}O_2$		2-*tert*-butyl-4-methoxymethyl-6-α-methylbenzylphenol					
	371.7	29.4	0	79.1	74.8	29.4	27.8
		5*A1+A4+A2+A3+4*A11+A12+7*A10+A31+A32					[101]
$C_{20}H_{26}O_3$		testosterone formate					
	398	26.36	0	66.22	66.2	26.36	26.4
	398.2	18.12	0	45.5	66.2	18.1	26.4
		4*A14+5*A15+2*A17+4*A16+2*A1+A37+A19+A18*B18+A114					[219, 396]
$C_{20}H_{28}O_2$		1-[3,5-di-*tert*-butyl-4-hydroxyphenyl]-5-hexyn-1-one					
	342.2	25.14	0	73.47	74.9	25.14	25.6
		6*A1+2*A4+2*A10+2*A11+2*A12+3*A2+A8+A9+A31+A35					[39]
$C_{20}H_{30}O_3Si_3$		1,1,3,3-tetraethyl-5,5-diphenylcyclotrisiloxane					
	279.1	18.37	0	65.84	97.9	18.37	27.3
		4*A1+4*A2+10*A10+2*A11+3*A112+3*A139+A14+3*A15					[216]
$C_{20}H_{32}$		10,10,13,13-tetramethylcyclohexadeca-1,5-diyne					
	323.2	18.83	0	58.25	63.8	18.83	20.6
		4*A1+A14+13*A15+2*A17+4*A20					[113]
$C_{20}H_{36}O_2$		1,10-cycloeicosanedione					
	327.2	55.06	0	168.28	98.7	55.06	32.3
		A14+17*A15+2*A112					[114]
$C_{20}H_{36}O_4$		1,9-cyclohexadecanedione bis ethylene ketal					
	404.2	42.13	0	104.24	91.4	42.13	36.9
		3*A14+15*A15+2*A17+4*A112					[114]
$C_{20}H_{40}$		1,1,9,9-tetramethylcyclohexadecane					
	364.2	25.1	0	68.93	82.6	25.1	30.1
		4*A1+A14+13*A15+2*A17					[112]

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)
$C_{20}H_{40}$		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]
$C_{20}H_{42}$		*n*-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-*n*-butoxy-4′-trifluoromethyldiphenyldiacetylene					
	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-*n*-pentyl-3′,4′-difluorodiphenyldiacetylene					
	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]
$C_{21}H_{24}O_3Si_3$		*cis*-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]
$C_{21}H_{24}O_3Si_3$		*trans*-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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{21}H_{30}O_4$	corticosterone					
454	33.32	0	73.39	84.1	33.32	38.7
	4*A14+5*A15+2*A17+5*A16+2*A1+2*A30*D30+A19+A18*B18+A114+A35+A2					[219]
$C_{21}H_{30}O_5$	hydrocortisone					
486	35.84	0	73.75	82.9	35.84	40.3
	4*A14+5*A15+3*A17+4*A16+2*A1+ 3*A30*E30+A19+A18*B18+A114+A35+A2					[219]
$C_{21}H_{35}N_3N_2$	N-palmitoyl-pyrazinamide					
362.7	51.82	0	142.87	192.5	51.82	69.8
	A1+14*A2*B2+3*A10+A12+2*A41+A71					[261]
$C_{21}H_{42}O$	11-heneicosanone					
336.7	76.2	0	226.31	207.7	76.2	69.9
	2*A1+A35+18*A2*B2					[262]
$C_{21}H_{42}O$	2-heneicosanone					
333.9	77.65	0	232.55	207.7	77.65	69.4
	2*A1+A35+18*A2*B2					[263]
$C_{21}H_{43}NO_3$	N-hexadecyl-L-valine					
349.1	29.1	83.36				
366.6	54.8	149.48	232.84	177.5	83.9	65.1
	3*A1+A3+A3*B3+15*A2*B2+A44+A36*B36					[249]
$C_{21}H_{43}NO_3$	N-hexadecyl-DL-valine					
375.1	80.5	0	214.61	177.5	80.5	66.6
	3*A1+A3+A3*B3+15*A2*B2+A44+A36*B36					[249]
$C_{21}H_{44}$	*n*-heneicosane					
305.7	15.48	50.65				
313.7	47.7	152.06	202.71	212.4	63.18	66.6
	19*A2*B2+2*A1					[216]
$C_{22}H_{12}$	1,12-benzoperylene					
554.2	17.37	0	31.34	43.2	17.37	24.0
	12*A10+4*A13+6*A12					[215]
$C_{22}H_{12}$	*o*-phenylenepyrene					
435.2	21.51	0	49.41	36.0	21.51	15.7
	A14+2*A15+5*A19+12*A10+2*A13+3*A12					[264]
$C_{22}H_{14}$	picene					
637.2	35.19	0	55.22	44.0	35.19	28.0
	14*A10+8*A12					[264]
$C_{22}H_{14}$	1,2:3,4-dibenzanthracene					
553.5	25.82	0	46.65	44.0	25.82	24.3
	14*A10+8*A12					[215]
$C_{22}H_{14}$	1,2:5,6-dibenzanthracene					
544.2	31.16	0	57.26	44.0	31.16	23.9
	14*A10+8*A12					[215]
$C_{22}H_{14}O_4$	1,4-bis(phenylglyoxaloyl)benzene					
425.1	32.3	0	75.98	92.2	32.3	39.2
	14*A10+4*A12+4*A35					[216]
$C_{22}H_{18}F_2O$	4-(6-hexenyloxy)-3′,4′-difluorodiphenyldiacetylene					
370	37.45	0	101.22	92.5	37.45	34.2
	A5+A6+4*A2+5*A12+7*A10+4*A9+2*A24+A32					[195]
$C_{22}H_{18}F_2O$	4-(*cis*-4-hexenyloxy)-3′,4′-difluorodiphenyldiacetylene					
364.4	35.32	0	96.93	90.9	35.32	33.1
	A1+2*A6+3*A2+5*A12+7*A10+4*A9+2*A24+A32					[195]
$C_{22}H_{18}F_2O$	4-(*cis*-3-hexenyloxy)-3′,4′-difluorodiphenyldiacetylene					
364.6	30.97	0	84.94	91.0	30.97	33.1
	A1+2*A6+3*A2+5*A12+7*A10+4*A9+2*A24+A32					[195]
$C_{22}H_{19}Br_2NO_3$	(S)-α-cyano-3-phenoxybenzyl (1R)-*cis*-3-(2,2-dibromovinyl)-2,2-dimethylcyclopropanecarboxylate					
372.9	40.71	0	109.18	96.6	40.71	36.0
	A14+A17+2*A16+2*A1+A6+A7+2*A21 +A38+A3*B3+A56+2*A12+A11+9*A10+A32					[221]
$C_{22}H_{24}O_3$	4-methyl-4-propyl-1,8-diphenyl-2,3,5-trioxabicyclo[4.3.0]non-7-ene					
351.2	16.6	0	47.27	60.1	16.6	21.1
	10*A10+A11+A12+2*A14+3*A15+A19+A18+A16+2*A17+A112+A113+2*A1+2*A2					[257]
$C_{22}H_{28}$	1,1′-diphenyl-1,1′-bicyclopentyl					
414	31.38	0	75.77	67.4	31.38	27.9
	2*A14+4*A15+2*A17+2*A11+10*A10					[289]

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)
$C_{22}H_{28}N_2O_2$		(4R*,5′R*,5′R*)-5,5-diphenyl-3,3′,4,4′-tetramethyl-2,2′-bioxazolidine					
	394	31.9	0	80.96	82.2	31.9	32.4
		2*A14+4*A15+6*A16+2*A119+10*A10+2*A11+4*A1+2*A112					[185]
$C_{22}H_{28}N_2O_2$		(2R*,3R*,6R*,7R*)-2,6-diphenyl-3,4,7,8-tetramethyl-*cis*-perhydro-[1,4]-oxazino-[3,2-*b*][1,4]-oxazine					
	368.8	20.9	0	54.03	82.2	20.9	31.8
		2*14+4*A15+6*A16+2*A119+10*A10+2*A11+4*A1+2*A112					[185]
$C_{22}H_{28}N_2O_2$		(2R*,3S*,6R*,7S*)-2,6-diphenyl-3,4,7,8-tetramethyl-*cis*-perhydro-[1,4]-oxazino-[3,2-*b*][1,4]-oxazine					
	379.4	18.4	0	48.5	82.2	18.4	31.2
		2*A14+4*A15+6*A16+2*A119+10*A10+2*A11+4*A1+2*A112					[185]
$C_{22}H_{28}O_3$		19-nor-17α-ethynyl-17β-acetoxy-4-androsten-3-one					
	480	27.3	0	56.88	62.2	27.3	29.9
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114+A38+2*A1+A8+A9					[216]
$C_{22}H_{29}FO_5$		dexamethasone					
	539	42.02	0	77.97	78.8	42.02	42.5
		4*A14+5*A15+2*A17+2*A17+4*A16+3*A1+3*A30*F30+A19					[219]
		+2*A18*B18+A18+A114+A35+A2+A27					
$C_{22}H_{30}O_3$		testosterone propionate					
	393	25.64	0	65.24	74.8	25.64	29.4
	393.2	22.13	0	56.3	74.8	22.1	29.4
		4*A14+5*A15+2*A17+4*A16+3*A1+A19+A18*B18+A114+A38+A2					[219, 396]
$C_{22}H_{40}O_4$		1,10-cyclooctadecanedione *bis* ethylene ketal					
	378.2	33.56	0	88.72	98.8	33.56	37.4
		3*A14+17*A15+2*A17+4*A112					[114]
$C_{22}H_{44}$		1,1,10,10-tetramethylcyclooctadecane					
	359.2	39.58	0	110.19	90.0	39.58	32.3
		A14+15*A15+4*A1+2*A17					[110]
$C_{22}H_{44}N_2O_2$		N,N′-di-*n*-hexylsebacamide					
	415	53.56	0	129.29	206.0	53.56	85.5
		18*A2*B2+2*A1+2*A60					[216]
$C_{22}H_{44}O_2$		butyl octadecanoate					
	288.4	2.22	7.7				
	299.7	37.48	125.05	132.75	220.1	39.7	66.0
		2*A1+A38+19*A2*B2					[79]
$C_{22}H_{44}O_2$		ethyl eicosanoate					
	313.5	15.58	49.68				
	396.7	7.78	19.62	69.3	220.1	23.36	87.3
		2*A1+A38+19*A2*B2					[216]
$C_{22}H_{44}O_4$		2,2,13,13-tetramethyl-1,3,10,12-tetraoxacyclododecane					
	374	61.9	0	165.51	109.7	61.9	41.0
		A14+19*A15+4*A112+2*A17+4*A1					[47]
$C_{22}H_{45}Br$		1-bromodocosane					
	303.8	23.14	76.15				
	317.2	44.98	141.8	217.95	231.1	68.12	73.3
		A1+21*A2*B2+A21					[265]
$C_{22}H_{45}NO$		N-hexyl hexadecanamide					
	343.1	57	0	166.13	213.9	57	73.4
		2*A1+19*A2*B2+A60					[217]
$C_{22}H_{45}NO_3$		N-hexadecyl-L-leucine					
	367.1	46.1	0	125.58	186.8	46.1	68.6
		3*A1+15*A2*B2+A3+A3*B3+A2*B2+A44+A36*B36					[249]
$C_{22}H_{45}NO_3$		N-hexadecyl-DL-leucine					
	333.1	4.3	12.91				
	355.1	60.6	170.66	183.57	186.8	64.9	66.3
		3*A1+15*A2*B2+A3+A3*B3+A2*B2+A44+A36*B36					[249]
$C_{22}H_{46}$		*n*-docosane					
	315.2	29.51	93.62				
	316.1	47.84	151.36	245.0	221.8	77.3	70.3
		2*A1+20*A2*B2					[227]
$C_{23}H_{15}ClO_3$		2-[(4-chlorophenyl)phenylacetyl]-1H-indene-13(2H)-dione					
	416.5	34.54	0	82.94	79.6	34.54	33.2
		A14+2*A15+2*A19+A16+13*A10+2*A114+A22*D22+A35+A12+					[221]
		2*A11+A3*B3					
$C_{23}H_{21}F_3O$		4-*n*-hexyloxy-4′-trifluoromethyldiphenyldiacetylene					
	394.8	33.98	0	86.07	91.0	33.98	35.9
		A1+5*A2+A11+3*A12+8*A10+4*A9+3*A25+A4*B4+A32					[195]
$C_{23}H_{22}O_6$		[2R-(2*a*,6*aa*,12*aa*)]-1,2,12,12a-tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-[1]benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6(6*a*H)-one (Rotenone)					

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	437.9	35.64	0	81.39	90.3	35.64	39.6
		3*A14+6*A15+2*A19+4*A19+3*A112+3*A16+					[221]
		A114+4*A10+2*A12+3*A1+2*A32+A5+A7					
$C_{23}H_{30}O_6$		prednisolone acetate					
	511	38.67	0	75.67	81.4	38.67	41.6
		4*A14+5*A15+3*A17+4*A16+3*A1+2*A30*E30+A19+					[219]
		2*A18*B18+A18+A114+A35+A2+A38					
$C_{23}H_{30}O_6$		cortisone acetate					
	509	38.43	0	75.5	78.8	38.43	40.1
		4*A14+5*A15+3*A17+3*A16+3*A1+2*A30*E30+A19+					[219]
		2*A18*B18+2*A114+A35+A2+A38					
$C_{23}H_{32}O_2$		3,3′-di-*tert*-butyl-5,5′-dimethyl-2,2-dihydroxydiphenylmethane					
	403.7	29.33	0	72.65	75.7	29.33	30.6
		8*A1+2*A4+6*A11+2*A12+A2+2*A31+4*A10					[101]
$C_{23}H_{32}O_3$		estra-1,3,5(10)-triene-3-o1-17β pentanoate					
	420.7	29.45	0	70	96.2	29.45	40.5
		3*A14+4*A15+2*A19+4*A16+A17+A38+A31+3*A10+A12+2*A1+3*A2					[137]
$C_{23}H_{32}O_3$		testosterone butyrate					
	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
		4*A14+5*A15+2*A17+4*A16+3*A1+A19+A18*B18+A114+A38+2*A2					[219, 396]
$C_{23}H_{32}O_4$		deoxycorticosterone acetate					
	430	29.66	0	68.98	79.4	29.66	34.1
		4*A14+5*A15+2*A17+4*A16+3*A1+A38+A19+A18*B18+A114+A35+A2					[219]
$C_{23}H_{32}O_6$		hydrocortisone acetate					
	496	36.95	0	74.49	87.0	36.95	43.2
		4*A14+5*A15+3*A17+4*A16+3*A1+2*A30*E30					[219]
		+A19+A18*B18+A114+A35+A2+A38					
$C_{23}H_{44}O_5$		1-aceto-3-stearin					
	319.9	41.69	0	130.31	222.5	41.69	71.2
		2*A1+16*A2*B2+A3*B3+2*A38+A30*B30+2*A2					[216]
$C_{23}H_{46}O$		12-tricosanone					
	342.2	78.03	0	228.04	226.4	78.03	77.5
		2*A1+A35+20*A2*B2					[19]
$C_{23}H_{46}O_2$		methyl docosanoate					
	325.0	82.3	0	251.7	228.9	82.3	74.6
		2*A1+A38+20*A2*B2					[391]
$C_{23}H_{48}$		*n*-tricosane					
	313.7	21.76	69.37				
	320.7	53.97	168.33	237.69	231.1	75.73	74.1
		2*A1+21*A2*B2					[227]
$C_{24}F_{50}$		perfluorodocosane					
	202.7	3.89	19.19				
	465.2	100.8	216.7	235.9	251.1	104.7	116.8
		44*A26+24*A4*B4+6*A25					[67]
$C_{24}H_{12}$		coronene					
	710.5	19.2	0	27.02	42.8	19.2	30.4
		12*A10+6*A12+6*A13					[215]
$C_{24}H_{14}$		1,2:4,5-dibenzopyrene					
	520.2	30.5	0	58.63	43.5	30.5	22.6
		14*A10+8*A12+2*A13					[215]
$C_{24}H14$		3,4:9,10-dibenzopyrene					
	556.8	27.87	0	50.05	42.5	27.87	24.2
		14*A10+8*A12+2*A13					[215]
$C_{24}H_{14}$		1,2:3,4-dibenzopyrene					
	501.2	24.68	0	49.24	42.5	24.68	21.8
		14*A10+8*A12+2*A13					[215]
$C_{24}H_{18}$		1, 3, 5-triphenylbenzene					
	446	33.4	0	74.89	88.6	33.4	39.5
		18*A10+6*A12					[132]
$C_{24}H_{18}$		*p*-quaterphenyl					
	233.0	0.41	1.78				
	587.2	37.8	64.37	66.15	88.6	38.2	52.0
		18*A10+6*A12					[157,215]
$C_{24}H_{28}O_2Si_3$		1,1,1,5,5,5-hexamethyl-3,3-diphenyltrisiloxane					
	270.5	22.75	0	84.12	88.6	22.75	24.0
		6*A1+2*A32+3*A109+10*A10+2*A11					[216]
$C_{24}H_{31}FO_5$		triamcinolone acetonide					

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)	
	566	45.29	0	80.02	78.6	45.29	44.5	
		5*A14+5*A15+5*A17+4*A16+4*A1+2*A30*F30					[219]	
		+A19+2*A18*B18+A18+A114+A35+A2+A28+2*A112						
$C_{24}H_{31}FO_6$		dexamethasome acetate						
	503	37.72	0	75	85.1	37.72	42.8	
		4*A14+5*A15+4*A17+4*A16+4*A1+2*A30*F30					[219]	
		+A19+2*A18*B18+A18+A114+A35+A2+A28+A38						
$C_{24}H_{32}$		1,1′-diphenyl-1,1′-bicyclohexyl						
	455	29.71	0	65.27	74.8	29.71	34.0	
		2*A14+6*A15+2*A17+2*A11+10*A10					[289]	
$C_{24}H_{34}$		1,1-diphenyldodecane						
	191	1.92	10.08					
	281.4	38.83	137.98	148.11	127.5	40.75	35.9	
		10*A10+10*A2+A1+2*A11+A3					[216]	
$C_{24}H_{34}O_3$		testosterone valerate						
	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	
		4*A14+5*A15+2*A17+4*A16+3*A1+A19+A18*B18+A114+A38+3*A2					[219, 396]	
$C_{24}H_{40}$		1-cyclohexyl-1-phenyldodecane						
	275.8	35.17	0	127.58	129.8	35.17	35.8	
		A14+3*A15+5*A10+A3+10*A2+A16+A1+A11					[216]	
$C_{24}H_{44}O_4$		1,11-cycloeicosanedione-*bis*-ethylene ketal						
	362.2	43.72	0	120.71	106.2	43.72	38.5	
		3*A14+19*A15+4*A112+2*A17					[114]	
$C_{24}H_{46}$		2,11-dicyclohexyldodecane						
	300.6	43.93	0	146.15	119	43.93	35.77	
		2*A14+2*A1+2*A16+8*A2+6*A15+2*A3					[216]	
$C_{24}H_{46}$		1,1-dicyclohexyldodecane						
	300.6	44.35	0	147.54	132.1	44.35	39.7	
		2*A14+2*A16+A1+10*A2+6*A15+A3					[216]	
$C_{24}H_{48}$		cyclotetraeicosane						
	297	38	127.95					
	322	10.8	33.54	161.49	111.1	48.8	35.8	
		21*A15+A14					[181]	
$C_{24}H_{48}O_2$		ethyl docosanoate						
	312.3	9.58	30.68					
	321.0	19.16	59.69	90.37	236.6	28.74	75.9	
		2*A1+A38+20*A2*B2+A2					[216]	
$C_{24}H_{50}$		*n*-tetracosane						
	321.3	31.3	97.42					
	324.1	54.89	169.37	266.79	240.4	86.19	77.9	
		22*A2*B2+2*A1					[216]	
$C_{25}H_{31}FO_8$		triamcinolone						
	543	42.56	0	78.39	86.6	42.56	47.0	
		4*A14+5*A15+4*A17+4*A16+2*A1+4*A30*F30					[219]	
		+A19+2*A18*B18+A18+A114+A35+A2+A28						
$C_{25}H_{34}O_3$		19-nor-17α-ethynyl-17β-(2,2-dimethylpropionoxy-4-androsten-3-one)						
	500	37.8	0	75.6	74.5	37.8	37.3	
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114					[216]	
		+A38+4*A1+A8+A9+A4*B4						
$C_{25}H_{40}O_2Si_2$		norethindrone pentamethyldisiloxy ether						
	355	22.9	0	64.51	80.1	22.9	28.4	
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114					[216]	
		+6*A1+A8+A9+2*A32+2*A109						
$C_{25}H_{46}O_6$		1,2-diaceto-3-sterin						
	208.3	45.56	0	218.72	229.7	45.56	47.8	
		3*A1+2*A2+3*A38+A3*B3+16*A2*B2					[216]	
$C_{25}H_{52}$		*n*-pentacosane						
	320.2	26.07	81.42					
	326.7	57.74	176.76	258.18	249.8	83.81	81.6	
		2*A1+23*A2*B2					[216]	
$C_{25}H_{52}$		5,5-bis(3,3-dimethylbutyl)-2,2,8,8-tetramethylnonane						
	472.7	48.53	0	102.67	93.8	48.53	44.4	
		4*(3*A1+A4+2*A2)+A4					[266]	
$C_{26}H_{14}$		1,12-phenyleneperylene						
	541.5	17.28	0	31.91	43.1	17.28	23.3	
		14*A10+8*A12+4*A13					[215]	
$C_{26}H_{18}$		9,9′-bifluorenyl						
	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		2*A14+4*A15+8*A19+2*A16+16*A10					[252]
$C_{26}H_{26}OSi_2$		1,3-dimethyl-1,1,3,3-tetraphenyldisiloxane					
	322.0	26.58	0	82.55	95.6	26.58	30.8
		20*A10+4*A11+2*A1+A32*C32+2*A109					[216]
$C_{26}H_{26}O_3Si_3$		dimethyltetraphenylcyclotrisiloxane					
	361.1	28.2	0	78.1	89.1	28.2	32.2
		A14+3*A15+3*A112+3*A139+2*A1+20*A10+4*A11					[216]
$C_{26}H_{38}$		2,3-dimethyl-2,3-bis(4-*tert*-butylphenyl)butane					
	493	43.93	0	89.11	57.4	43.93	28.3
		4*A11+10*A1+4*A4+8*A10					[289]
$C_{26}H_{46}$		11-phenyleicosane					
	294.3	64.77	0	220.08	187.3	64.77	55.1
		2*A1+17*A2*B2+A3+5*A10+A11					[290]
$C_{26}H_{52}$		11-cyclohexyleicosane					
	269.9	48.7	0	180.44	189.6	48.7	51.2
		A14+A16+2*A1+9*A2*B2+3*A15+A3+8*A2					[290]
$C_{26}H_{52}$		1,1,4,4,10,10,13,13-octamethylcyclooctadecane					
	427.2	6.74	15.77				
	438.2	20.17	46.02	61.79	91.2	26.9	40.0
		A14+15*A15+8*A1+4*A17					[107, 116]
$C_{26}H_{52}O_2$		ethyl tetracosanate					
	317.7	11.2	35.27				
	327.4	22.94	70.07	105.34	255.2	34.14	83.6
		2*A1+22*A2*B2+A38+A2					[216]
$C_{26}H_{53}NO$		N-decyl hexadecanamide					
	333	5	15.02				
	347	63	181.56	196.57	251.2	68	87.2
		2*A1+23*A2*B2+A60					[260]
$C_{26}H_{54}$		*n*-hexacosane					
	326.5	32.2	98.7				
	329.5	59.5	180.6	289.3	259.1	95.3	85.3
		2A1+24*A2*B2					[216]
$C_{27}H_{30}O_3$		19-nor-17α-ethynyl-17β-(benzoyloxy-4-androsten-3-one)					
	531	41.5	0	78.15	74.2	41.5	39.4
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114+A38+A1+ 5*A10+A12+A8+A9					[216]
$C_{27}H_{32}O_3$		spiro[8.5.0(3,7)]-3,5-diphenyl-1,2,8-trioxa-10,12-tetramethyltetradec-5-ene					
	389.2	15	0	38.54	52.7	15	20.5
		3*A14+5*A15+4*A17+10*A10+A11+A12+4*A1+A19+A18+A16+A113+A112					[257]
$C_{27}H_{38}O_3$		19-nor-17*a*-ethynyl-17*b*-(heptanoyloxy-4-androsten-3-one)					
	340	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					[216]
$C_{27}H_{46}O$		cholesterol					
	304.8	2.5	8.2				
	420.2	27.41	65.22	73.42	73.7	29.91	31.0
		4*A14+5*A15+5*A16+2*A17+5*A1+3*A2+2*A3+A30+A19+A18					[216, 388]
$C_{27}H_{54}N_6$		*tris* N,N-diisobutylamino-1,3,5-triazine					
	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					[267]
$C_{27}H_{56}$		*n*-heptacosane					
	318	2.26	7.11				
	325.4	26.28	80.75				
	332.1	59.05	177.82	265.68	268.4	87.59	89.2
		2*A1+25*A2*B2					[268]
$C_{28}H_{16}$		1,2,4,5,8,9-tribenzopyrene					
	608	28.8	0	47.37	43.4	28.8	26.4
		16*A10+10*A12+2*A13					[264]
$C_{28}H_{28}O_2P_2$		1,4-*bis*(diphenylphosphino)butane					
	405.9	45.3	0	111.6	105.4	45.3	42.8
		2*A72+20*A10+4*A12+4*A2					[269]
$C_{28}H_{32}O_4Si_4$		1,1,3,3-tetramethyl-5,5,7,7-tetraphenylcyclotetrasiloxane					
	186.5	0.24	1.3				
	271.5	1.05	3.85				
	346.2	27.05	78.13	83.29	98.2	28.34	34.0
		4*A1+20*A10+4*A11+4*A139+4*A112+A14+5*A15					[216]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{28}H_{32}O_4Si_4$		1,1,5′,7′-tetramethyl-1′,3′,5,7-tetraphenylcyclotetrasiloxane					
	373.4	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]
$C_{28}H_{40}$		1,1′-diphenyl-1,1′-bicyclooctyl					
	432	35.98	0	83.26	89.6	35.98	38.7
		2*A14+10*A15+2*A17+2*A11+10*A10					[289]
$C_{28}H_{56}$		1,1,5,5,11,11,15,15-octamethylcycloeicosane					
	439.2	47.7	0	108.6	98.6	47.7	43.3
		A14+17*A15+8*A1+4*A17					[107]
$C_{28}H_{56}O_2$		ethyl hexaconsanate					
	322.7	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]
$C_{28}H_{58}$		*n*-octacosane					
	331.3	35.44	106.98				
	334.5	64.64	193.28	300.26	277.8	100.08	92.9
		26*A2*B2+2*A1					[216]
$C_{29}H_{35}FO_{10}$		triamcinolone diacetate					
	508	38.31	0	75.42	98.7	38.31	50.1
		4*A14+5*A15+4*A17+4*A16+6*A1+A19					[219]
		+2*A18*B18+A18+A114+A35+A2+A28+4*A38					
$C_{29}H_{44}O_2$		3,3′,5,5′-tetra-*tert*-butyldiphenylmethane-4,4′-diol					
	447.7	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]
$C_{29}H_{60}$		*n*-nonacosane					
	331.4	29.71	89.65				
	336.6	66.11	196.43	286.08	287.1	95.81	96.6
		2*A1+27*A2*B2					[216]
$C_{30}H_{46}$		3,4-diethyl-3,4-bis(4-*tert*-butylphenyl)hexane					
	400	29.71	0	74.27	85.9	29.71	34.4
		10*A1+4*A4+4*A11+8*A10+4*A2					[289]
$C_{30}H_{46}O_2S$		*bis*-[3,5-di-*tert*-butyl-4-hydroxybenzyl]sulfide					
	417.2	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]
$C_{30}H_{60}O_4$		2,2,6,6,9,9,13,13,17,17,20,20-dodecamethyl-1,3,12,14-tetraoxacyclodocosane					
	406.4	57.3	0	141	112.1	57.3	45.5
		A14+19*A15*+4*A112+6*A17+12*A1					[47]
$C_{30}H_{60}$		1,1,4,4,12,12,15,15-octamethylcyclododocosane					
	411.2	58.58	0	142.45	106.0	58.58	43.6
		A14+19*A15+4*A17+8*A1					[107]
$C_{30}H_{61}Br$		1-bromotricosane					
	313.2	23.85	76.15				
	339.6	79.5	234.09	310.24	305.7	103.34	103.8
		A1+29*A2*B2+A21					[265]
$C_{30}H_{62}$		triacontane					
	335.3	37.49	111.82				
	338.7	68.83	203.24	315.06	296.4	106.32	100.4
		2*A1+28*A2*B2					[216]
$C_{31}H_{44}O_2$		3,3′-*bis*-(1-cyclohexylethyl)-5,5′-dimethyldiphenylmethane-2,2′-diol					
	400.7	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					[101]
		+6*A15+2*A16+A2					
$C_{31}H_{64}$		11-*n*-decylheneicosane					
	282.3	71.13	0	251.96	288.3	71.13	81.4
		3*A1+27*A2*B2+A3					[216]
$C_{32}H_{14}$		ovalene					
	729	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]
$C_{32}H_{39}ClO_2$		norethindrone-6-(4-chlorophenyl)hexanoate					
	413	28.8	0	69.73	109.1	28.8	45.0
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114+					[216]
		A38+A1+4*A10+A11+A12+A8+A9+5*A2+A22*B22					
$C_{32}H_{64}O_2$		ethyl triacontanoate					
	334.7	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]
$C_{32}H_{64}O_4$		2,2,6,6,10,10,14,14,18,18,22,22-dodecamethyl-1,3,13,15-tetraoxacyclotetracosane					
	342.5	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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
		A14+21*A15+4*A112+6*A17+12*A1					[47]
$C_{32}H_{66}$		dotriacontane					
	338.7	41.38	122.18				
	343.5	76.57	222.93	345.11	315.1	117.94	108.2
		2*A1+30*A2*B2					[216]
$C_{33}H_{34}O_3$		norethindrone-biphenyl-4-carboxylate					
	462	31.6	0	68.4	88.8	31.6	41.0
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114+A38+A1+9*A10+3*A12+A8+A9					[216]
$C_{33}H_{40}O_3$		norethindrone-4-cyclohexybenzoate					
	482	38.6	0	80.08	87.0	38.6	41.9
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114+A38					[216]
		+A1+4*A10+A11+A12+A14+3*A15+A16+A8+A9					
$C_{33}H_{48}O_3$		norethindrone-*trans*-3-(4-butylcyclohexyl)propionate					
	374	22.5	0	60.16	112.9	22.5	42.2
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114+A38					[216]
		+A1+A14+3*A15+2*A16+A1+3*A2+2*A2+A8+A9					
$C_{33}H_{48}O_3^*$		norethindrone-*trans*-4-hexylcyclohexylcarboxylate					
	398	22.6	0	56.78	112.9	22.6	44.9
		4*A14+5*A15+4*A16+A19+2*A17+A18*B18+A114					[216]
		+A38+A1+A14+3*A15+2*A16+5*A2+A1+A8+A9					
$C_{33}H_{68}$		triatriacontane					
	344	105.0	0	305.2	324.4	105.0	111.6
		2*A1+31*A2*B2					[216]
$C_{34}H_{54}$		4,5-dipropyl-4,5-bis(4-*tert*-butylphenyl)octane					
	419	40.58	0	96.86	114.4	40.58	47.9
		4*A4+4*A11+10*A1+8*A2+8*A10					[289]
C_3H_{70}		tetratriacontane					
	341.5	29.3	85.8				
	345.9	79.96	231.1	316.96	333.7	109.24	115.4
		2*A1+32*A2*B2					[217]
$C_{35}H_{72}$		*n*-pentatriacontane					
	344.7	41.09	119.2				
	347.2	86.4	248.85	368.04	343.1	127.49	119.1
		2*A1+33*A2*B2					[216]
$C_{36}H_{18}$		decacyclene					
	666	25.4	0	38.14	49.4	25.4	32.9
		3*A14+6*A15+15*A19+3*A12+18*A10					[264]
$C_{36}H_{24}$		1,3,5-tri-α-naphthylbenzene					
	472	42.26	0	89.53	88.2	42.26	41.6
		24*A10+12*A12					[56]
$C_{36}H_{46}O_4$		4′,4′-didecanoyloxydiphenyldiacetylene					
	308	44.9	145.78				
	403	42.2	104.71	250.49	183.0	42.2	73.7
		8*A10+4*A12+4*A9+2*A38+16*A2+2*A1					[216]
$C_{36}H_{74}$		hexatriacontane					
	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
		2*A1+34*A2*B2					[216]
$C_{38}H_{50}O_4$		4,4′-diundecanoyloxydiphenyldiacetylene					
	339	18.1	53.39				
	358	7.59	21.14				
	399	36.2	90.73	165.26	197.2	61.59	78.7
		8*A10+4*A12+4*A9+2*A38+18*A2+2*A1					[216]
$C_{38}H_{62}$		5,6-dibutyl-5,6-bis(4-tert-butylphenyl)decane					
	386	43.1	0	111.65	143.0	43.1	55.2
		4*A4+4*A11+10*A1+12*A2+8*A10					[289]
$C_{39}H_{74}O_6$		glyceryl trilaurate					
	319.5	123.51	0	386.57	360.3	123.51	115.1
		3*A1+30*A2*B2+2*A2+A3*B3+3*A38					[216]
$C_{40}H_{54}O_4$		4,4′-didodecanoyloxydiphenyldiacetylene					
	374	50.2	134.22				
	401	44	109.73	243.95	255.4	94.2	102.4
		8*A10+4*A12+4*A9+2*A38+20*A2*B2+2*A1					[216]
$C_{40}H_{82}$		tetracontane					
	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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{42}H_{66}O_{12}$		benzene-hexa-*n*-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
		6**A*12+6**A*38+6**A*1+24**A*2					[216]
$C_{45}H_{86}O_6$		glyceryl trimyristate					
	330.2	152.2	0	460.92	416.3	152.2	137.5
		3**A*1+36**A*2**B*2+2**A*2+*A*3**B*3+3**A*38					[216]
$C_{51}H_{98}O_6$		glyceryl tripalmitate					
	338.9	179.37	0	529.27	472.3	179.37	160.1
		3**A*1+42**A*2**B*2+2**A*2+*A*3**B*3+3**A*38					[216]
$C_{51}H_{100}ClN_5$		2,4-*bis*-N,N-didodecylamino-6-chloro-1,3,5-triazine					
	307.5	34.25	0	111.4	441.0	34.25	135.6
		4**A*1+44**A*2**B*2*+2**A*43+*A*22**F*22+3**A*12+*A*41					[267]
$C_{51}H_{102}N_6$		tris N,N-dioctylamino-1,3,5-triazine					
	312.7	74.25	0	237.45	440.9	74.25	137.9
		6**A*1+42**A*2**B*2+3**A*41+3**A*43+3**A*12					[267]
$C_{57}H_{110}O_6$		glyceryl tristearate					
	345.7	203.26	0	587.97	532.6	203.26	184.1
		3**A*1+48**A*2**B*2+2**A*2**B*2+*A*3**B*3+3**A*38					[216]
$C_{60}H_{78}Sn_2O$		hexakis(2-methyl-2-phenylpropyl)distanoxane					
	417.7	71.81	0	171.92	165.8	71.81	69.3
		12**A*1+6**A*2+6**A*4+30**A*10+6**A*11+2**A*110+*A*32					[221]
$C_{60}H_{122}$		hexacontane					
	373.2	186.8	0	500.41	576.4	186.8	215.1
		2**A*1+58**A*2**B*2					[268]
$C_{63}H_{126}N_6$		*tris* N,N-didecylamino-1,3,5-triazine					
	314.4	87.68	0	278.88	434.2	87.68	136.5
		6**A*1+54**A*2+3**A*41+3**A*43+3**A*12					[267]
$C_{75}H_{150}N_6$		*tris* N,N-didodecylamino-1,3,5-triazine					
	320.3	119.19	0	372.12	519.8	119.19	166.5
		6**A*1+66**A*2+3**A*41+3**A*43+3**A*12					[267]
$C_{78}H_{108}$		2,3,6,7,10,11-*hexakis*(1-decynyl)triphenylene					
	314.2	63	0	200.54	326.6	63	102.6
		6*7**A*2+6**A*1+6*2**A*9+6**A*10+12**A*12					[216]

[a]Units for $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ 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 amphiphillic 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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta T_0^{T_{fus}} H_{tpce}$ (calcd)
CF_2*		poly(tetrafluoroethylene)					
	297	850	2.86				
	605	4100	6.78	9.64	9.83	4.95	5.95
		*A*4**B*4 + 2**A*26					[389]
CH_2*		poly(ethylene)					
	414.6	4.11	0	9.91	8.4	4.11	3.86
		*A*2**B*2					[389]
CH_2O*		poly(oxymethylene)					
	457.5	9.79	0	21.4	14.0	9.79	6.41
		*A*2**B*2 + *A*32					[389]
C_2ClF_3*		poly(chlorotrifluoroethylene)					
	493	5.02	0	10.2	15.8	5.02	7.8
		2**A*4**B*4 + 2**A*26 + *A*27 + *A*22**F*22					[389]
C_3HF_3*		poly(trifluoroethylene)					
	495.2	5.44	0	11.0	12.4	5.44	6.3
		2**A*4**B*4 + 2**A*26 + *A*27					[389]
$C_2H_2F_2$*		poly(vinylidene fluoride)					
	483	6.70	0	13.9	16.9	6.7	8.18
		*A*2 + *A*4**B*4 + 2**A*26					[389]
$C_2H_2O_2$*		poly(glycolic acid)					
	501	9.74	0	19.4	17.0	9.74	7.4
		*A*2**B*2 + *A*38					[389]
C_2H_3Cl*		poly(vinylchloride)					
	546	11.0	0	20.1	13.5	11.0	7.3
		*A*2 + *A*3**B*3 + *A*22**C*22					[389]
C_2H_3F*		poly(vinylfluoride)					
	473	7.54	0	15.0	10.0	7.54	5.0
		*A*2 + *A*3**B*3 + *A*27					[389]
C_2H_4O*		poly(oxyethylene)					
	342	8.66	0	25.3	23.3	8.66	8.0
		2**A*2**B*2 + *A*32					[389]
C_2H_4O*		poly(vinyl alcohol)					
	538	711	0	13.2	13.8	7.11	7.4
		*A*2 + *A*3**B*3 + *A*30**C*30					[389]
$C_2H_4O_2$*		poly(glycolide)					
	501	11.75	0	23.5	17.0	11.75	8.5
		*A*3**B*3 + *A*38					[216]
C_3H_3N*		poly(acrylonitrile)					
	590	5.0	0	8.5	15.0	5.0	8.8
		*A*2 + *A*3**B*3 + *A*56					[390]
$C_3H_4O_2$*		poly(β-propiolactone)					
	366	10.9	0	29.8	26.3	10.9	9.6
		2**A*2**B*2 + *A*38					[389]
C_3H_6*		poly(propylene)					
	460.7	8.70	0	18.9	8.3	8.7	3.8
		*A*1 + *A*2 + *A*3					[389]
C_3H_6O*		poly(propyleneoxide)					
	348	8.40	0	24.1	19.6	8.4	6.8
		*A*1 + *A*2 + *A*3**B*3 + *A*32					[389]
C_3H_6O*		poly(trimethyleneoxide)					
	308	9.44	0	30.6	32.6	9.44	10.0
		3**A*2**B*2 + *A*32					[389]
$C_3H_6O_2$*		poly(oxymethylenoxyethylene)					
	328	16.7	0	50.9	35.1	16.7	11.5
		2**A*2**B*2 + *A*2 + 2**A*32					[389]
$C_4H_3F_3O_2$*		poly(vinyl trifluoroacetate)					
	448	7.5	0	16.7	31.2	7.5	14.0
		*A*2 + *A*3**B*3 + *A*4**B*4 + *A*38 + 3**A*25					[390]
$C_4H_4O_4$*		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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta T_0^{T_{fus}} H_{tpce}$ (calcd)
	450	23.0	0	51.1	34.0	23.0	15.3
		2A2*B2+2*A38					[389]
$C_4H_4O_2$*		poly(γ-butyrolactone)					
	337.5	14.0	0	41.5	35.6	14.0	12.0
		3*A2*B2+A38					[389]
C_4H_5Cl*		*trans*-poly(chloroprene)					
	368	8.4	0	22.8	25.0	8.4	9.2
		2*A2+A6+A7+A22*C22					[390]
C_4H_6*		*cis*-poly(1,4-butadiene)					
	284.7	9.2	0	32.3	29.2	9.2	8.3
		2*A2+2*A6					[389]
C_4H_6*		*trans*-poly(1,4-butadiene)					
	356	7.8	21.9				
	437	3.73	8.5	30.5	29.2	11.5	12.8
		2*A2+2*A6					[389]
C_4H*		poly(1-butene)					
	411	7.0	0	17.0	15.4	7.0	6.3
		A1+2*A2+A3					[389]
C_4H_8*		poly(isobutylene)					
	317	12.0	0	37.9	7.5	12.0	2.4
		2A1+A2+A4					[389]
C_4H_8O*		poly(oxytetramethylene)					
	330	14.4	0	43.6	41.9	14.4	13.8
		4*A2*B2+A32					[389]
C_5H_8*		*cis*-poly(isoprene)					
	301.2	4.35	0	14.4	26.4	4.35	8.0
		A1+2*A2+A6+A7					[389]
C_5H_8*		*trans*-poly(isoprene)					
	347	12.8	0	36.9	26.4	12.8	9.2
		A1+2*A2+A6+A7					[389]
$C_5H_8Cl_2O$*		poly(2,2-bis(chloromethyl)trimethylene-3-oxide)					
	463	32.0	0	69.1	30.7	32.0	14.2
		4*A2+A4+2*A22*D22+A32					[389]
$C_5H_8O_2$*		poly(methyl methacrylate)					
	450	9.5	0	21.1	27.0	9.5	12.2
		2*A1+A2+A4*B4+A38					[389]
$C_5H_8O_2$*		poly(2,2-dimethylpropiolactone)					
	513	14.9	0	29.0	18.4	14.9	13.9
		2*A1+A2+A4*B4+A38					[389]
C_5H_{10}*		poly(1-pentene)					
	403.2	6.3	0	15.6	26.9	6.3	10.8
		A1+2*A2*B2+A3					[389]
$C_5H_{10}O_2$*		poly(oxymethyleneoxytetramethylene)					
	296	14.3	0	48.3	53.7	14.3	15.9
		A2+2*A2*B2+2*A32					[389]
C_6H_4O*		poly(oxy-1,4-phenylene)					
	535	7.82	0	14.6	19.3	7.8	10.3
		4*A10+2*A12+A32					[389]
C_6H_4S*		poly(thio-1,4-phenylene)					
	593	8.65	0	14.6	15.4	8.65	9.1
		4*A10+2*A12+A84					[389]
$C_6H_{10}O_2$*		poly(ε-caprolactone)					
	342.2	17.9	0	52.3	54.2	17.9	18.5
		4*A2*B2+A38					[389]
$C_6H_{10}O_2$*		poly(isopropyl acrylate)					
	421	5.9	0	14.0	30.3	5.9	12.8
		2*A1+2*A3*B3+A2+A38					[389]
$C_6H_{11}NO$*		nylon-6 (poly(6-aminohexanoic acid))					
	533	26.0	0	48.8	48.0	26.0	25.6
		5*A2*B2+A61					[389]
C_6H_{12}*		poly(4-methyl-1-pentene)					
	523	10.0	0	19.0	16.6	10.0	8.7
		2A1+2*A2+A3					[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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta T_0^{T_{fus}} H_{tpce}$ (calcd)
C_8H_8*		poly(styrene)					
	516.2	10.0	0	19.4	18.1	10.0	9.3
		$A2+A3+5*A10+A11$					[389]
C_8H_8*		poly(xylylene)					
	504	5.0	9.9				
	560	1.5	2.7				
	700	10.0	14.0	26.6	24.6	16.5	17.5
		$4*A10+2*A11+2*A2$					[389]
C_8H_8O*		poly(2,6-dimethyl-1,4-diphenylene oxide)					
	580	5.95	0	10.3	20.5	5.95	11.9
		$2*A1+2*A10+2*A11+2*A12+A32$					[389]
$C_8H_{12}O_4$*		polyester-2,6 (poly(ethylene adipate))					
	320	15.9	0	49.7		15.9	
	338	21.0	0	62.1	66.8	21.0	22.6
		$4*A2*B2+2*A2+2*A38$					[389]
$C_8H_{16}O$*		poly(oxyoctamethylene)					
	347	29.3	0	84.4	79.1	29.3	27.5
		$8*A2*B2+A32$					[389]
$C_{10}H_8O_4$*		poly(ethylene terephthalate)					
	553	26.9	0	48.6	44.2	26.9	24.4
		$2*A2+4*A10+2*A12+2*A38$					[389]
$C_{11}H_{20}O_2$*		poly(undecanolactone)					
	365	39.5	0	108.2	100.7	39.7	36.8
		$10*A2*B2+A38$					[389]
$C_{11}H_{21}NO$*		nylon-11 (poly(11-aminoundecanoic acid))					
	493	44.7	0	90.7	94.5	44.7	46.6
		$10*A2*B2+A61$					[389]
$C_{12}H_{12}O_4$*		poly(tetramethylene terephthalate)					
	518	32.0	0	61.8	58.4	32.0	30.3
		$4*A2+4*A10+2*A12+2*A38$					[389]
$C_{12}H_{20}O_4$*		polyester-2,10 (poly(ethylene decanedioate))					
	356.2	31.9	0	89.6	104.0	31.9	37.0
		$8*A2*B2+2*A2+2*A38$					[389]
$C_{12}H_{22}N_2O_2$*		nylon-6,6,α (poly(hexamethylene hexanediamide))					
	574	57.8	0	100.6	96.0	57.8	55.1
		$10*A2*B2+A61$					[389]
$C_{12}H_{23}NO$*		poly(12-aminododecanoic acid)					
	500	48.4	0	96.8	103.8	48.4	51.9
		$11*A2*B2+A61$					[389]
$C_{13}H_{24}O_2$*		poly(tridecanolactone)					
	368	50.6	0	137.5	119.3	50.6	43.9
		$12*A2*B2+A38$					[389]
$C_{14}H_{10}O_4$*		poly(ethylene naphthalene-2,6-dicarboxylate)					
	610	25.0	0	41.0	44.0	25.0	26.8
		$2*A2+6*A10+2*A12+2*A38$					[389]
$C_{14}H_{16}O_4$*		poly(hexamethylene terephthalate)					
	434	35.0	0	80.6	72.6	35.0	31.5
		$6*A2+4*A10+2*A12+2*A38$					[389]
$C_{15}H_{28}N_2O_2$*		nylon-6,9 poly(hexamethylene nonanediamide)					
	500	69.0	0	138.0	123.9	69.0	62.0
		$14*A2*B2+2*A61$					[389]
$C_{15}H_{28}O_2$*		poly(pentadecanolactone)					
	370.5	63.4	0	171.1	139.7	63.4	51.1
		$14*A2*B2+A38$					[389]
$C_{16}H_{28}O_4$*		poly(decamethylene adipate)					
	343	42.7	0	124.4	145.6	42.7	49.9
		$14*A2*B2+2*A38$					[389]
$C_{16}H_{30}N_2O_2$*		nylon-6,10 (poly(hexamethylene decanediamide))					
	506	71.7	0	141.6	133.2	71.7	67.4
		$14*A2*B2+2*A61$					[389]
$C_{18}H_{12}O$*		poly(oxy-2,6-diphenyl-1,4-diphenylene)					
	753	12.2	0	16.2	48.5	12.2	36.5
	770	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta T_0^{T_{fus}} H_{tpce}$ (calcd)
	12**A*10+6**A*12+*A*32						[389, 390]
$C_{18}H_{32}O_4$*		polyester-9,9 (poly(nonamethylene nonanedioate))					
338		43.2	0	127.8	164.2	43.2	55.5
	16**A*2**B*2+2**A*38						[389]
$C_{18}H_{24}O_4$*		poly(decamethylene terephthalate)					
411		46.1	0	112.1	123.0	46.1	50.6
	10*A*2**B*2+4**A*10+2**A*38						[389]
$C_{18}H_{32}N_2O_2$*		nylon-6,12 (poly(hexamethylene dodecanediamide))					
520		80.1	0	154.0	151.8	80.1	78.9
	16**A*2**B*2+2**A*61						[389]
$C_{19}H_{12}O_3$*		poly(oxy-1,4-phenylene-oxy-1,4-phenylene-carbonyl-1,4-phenylene)					
668.2		37.4	0	56.0	57.8	37.4	38.6
	12**A*10+6**A*12+2**A*32+*A*35						[389]
$C_{20}H_{36}O_4$*		poly(decamethylene-sebacate)					
353		50.2	0	142.2	182.8	50.2	64.5
	18**A*2**B*2+2**A*38						[389]

[a]These 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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
CBr_2Cl_2		dibromodichloromethane					
	258.8	5.4	21.0				
	294.4	2.3	7.9	28.8	44.4	7.7	13.1
		$A4*B4+2*A21+2*A22*D22$					[311]
$CHBr_3$		tribromomethane					
	281.5	11.1		39.4	42.7	11.1	12.0
		$A3*B3+3*A21$					[364]
CH_2O*		formic acid					
	281.4	12.68		45.1		12.7	
		Group value not available					[216]
CH_2F_2		difluoromethane					
	136.4	4.4		32.0	39.9	4.4	5.4
		$A2+2*A26$					[306]
CH_2I_2		diiodomethane					
	279.2	12.1		43.2	45.9	12.1	12.8
		$A2+2*A29$					[364]
CH_3Br		bromomethane					
	179.5	6.0		33.3	35.1	6.0	6.3
		$A1+A21$					[364]
CH_3I		iodomethane					
	206.8	9.1		44.1	37.0	9.1	7.7
		$A1+A29$					[367]
CH_4^*		methane					
	90.7	0.94		10.4		0.94	
		Group value not available					[216]
CH_4N_2O*		urea					
	408.1	12.9		31.7		12.9	
	406.5	14.8		36.4		14.8	
	406	14.5		35.7		14.5	
		Group value not available					[138, 216]
CH_4N_2S*		thiourea					
	452.2	12.6		27.8		12.6	
		Group value not available					[27]
CH_6BrN		methylammonium bromide					
	397.7	1.6	4.0				
	488.4	3.51	7.2				
	531.9	8.34	15.7	26.9		11.85	
		Group value not available					[216]
COS*		carbonyl sulfide					
	134.3	4.73		35.2		4.73	
		Group value not available					[216]
CS_2*		carbon disulfide					
	161.1	4.39		27.2		4.39	
		Group value not available					[216]
CSe_2*		carbon diselenide					
	229.5	6.36		27.7		6.36	
		Group value not available					[216]
$C_2Cl_3F_3$*		1,1,1-trichlorotrifluoroethane					
	287.5	4.11		14.3		4.11	
		Forms plastic crystal					[216]
$C_2Cl_4F_2$*		1,1,1,2-tetrachlorodifluoroethane					
	314.2	4.0		12.7	51.7	4.0	16.2
		$4*A22*F22+2*A26+2*A4*B4$					[216]
C_2F_4O*		trifluoroacetyl fluoride					
	113.7	4.87		42.8		4.7	
		Group value not available					[216]
$C_2F_2O_2$*		oxalyl fluoride					
	260.7	13.4		51.4		13.4	
		Group value not available					[216]
C_2HF_5		pentafluoroethane					
	172.6	2.25		13.0	39.9	2.3	6.8

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

	T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		$A4*B4+A3*B3+3*A25+2*A26$					[306]
C_2H_2		acetylene					
	142.7	2.54	17.8				
	192.4	3.76	19.5	37.3	29.8	6.3	5.7
		$2*A8$					[322]
$C_2H_2AsCl_3$		*trans*-β-(chlorovinyl)dichloroarsine					
	270.7	17.1		63.2	50.1	17.1	13.6
		$A98+2*A6*B6+3*A22*D22$					[369]
$C_2H_3N_3O_3$		1,1,1-trinitroethane					
	311.7	4.6	14.77				
	329.2	11.7	35.60	50.4	47.7	16.3	15.8
		$A1+3*A50+A4*B4$					[329, 352]
$C_2H_3N_3O_7$		2,2,2-trinitroethanol					
	312.5	18.0	57.6				
	344.9	2.7	7.9	65.5	59.5	20.7	20.5
		$A2+3*A50+A30*D30+A4*B4$					[352]
C_2H_6Cd*		dimethylcadmium					
	254.4	1.52	5.98				
	270.5	7.84	29.0	35.0	33.2	9.36	9.0
		$2*A1+A114$					[328]
$C_2H_8BF_4N$*		dimethylammonium tetafluoroborate					
	283.5	7.5	26.5				
	375	3.5	9.3	35.8		11.0	
		Group value not available					[216]
C_2H_8BrN*		ethylammonium bromide					
	369.9	12.1	32.6				
	439.5	8.5	19.4	52.0		20.6	
		Group value not available					[216]
C_2N_2*		cyanogen					
	245.3	8.11		33.1		8.11	
		Group value not available					[216]
$C_3H_4N_4O_6$*		1,3,3-trinitroazetidine					
	375.5	30.3		80.7		30.3	
							[303, 332]
$C_3H_6N_2O_5$		2,2-dinitropropanol					
	281.7	15.06	53.5				
	366.7	2.85	7.8	61.2	53.7	17.9	19.7
		$A1+A2+A4*B4+2*A50+A30*C30$					[352]
$C_3H_6N_2O_7$*		2,2-dinitro-1,3-propanediol					
	341.2	21.34		62.5	71.7	21.34	24.3
		$2*A2+2*A50+2*A30*D30+A4*B4$ (Decomposes before melting)					[352]
C_3H_9In*		trimethylindium					
	358.7	14.3		39.9	33.5	14.3	12.0
		$3*A1+A105$					[304]
C_3H_9Tl*		trimethylthallium					
	311.2	16.74		53.8	53.8	16.7	16.7
		$3*A1+A143$					[370]
$C_3H_{10}BrN$*		propylammonium bromide					
	464.6	13.3		28.7		13.3	
		Group value not available					[216]
C_4F_8S*		octafluorotetrahydrothiophene					
	146.0	10.88	74.5				
	266.7	2.09	7.8	82.4	45.3	13.0	12.1
		$A14+8*A28+4*A17+2*A15+A131$					[317]
$C_4H_3Cl_3OS$*		methyl trichlorothioacrylate					
	286.25	20.4		71.2		20.4	
		Group value not available					[216]
C_4H_4Se*		selenophene					
	122.7	0.3	2.5				
	192.8	1.11	5.73				
	240.2	4.58	19.1	27.3		6.0	
		Group value not available					[216]
$C_4H_6O_6$*		D-tartaric acid					
	445.1	32.3		72.6	85.2	32.3	37.9
		$2*A3*B3+2*A30*D30+2*A36*D36$					[392]
$C_4H_6O_2$		vinyl acetate					
	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		$A1+A5+A6+A38$					[353]
$C_4H_6O_3$		*p*-dioxanone					
	301.7	16.14		53.5	48.8	16.1	14.7
		A14+3*A15+A115+A112					[338]
C_4H_6O*		cyclobutanone					
	220.5	10.8		48.8	35.7	10.8	7.9
		$A14+A15+A114$					[393]
$C_4H_{10}Te$*		diethyl telluride					
	161.5	7.62		47.2	47.2	7.6	7.7
		$2*A1+2*A2+A140$					[299]
$C_4H_{11}AsO_2$*		diethylarsinic acid					
	411	19.9		48.3	25.4	19.9	10.4
		$2*A1+2*A2+A142$					[381]
C_5F_{10}		perfluorocyclopentane					
	118.2	5.0	41.9				
	238.5	3.0	12.6	54.5	42.8	8.0	12.1
		$A14+2*A15+10*A28+5*A17$					[335]
C_5F_{12}		perfluoro-*n*-pentane					
	147.8	6.8		46.0	63.4	6.8	9.3
		$6*A25+6*A26+5*A4*B4$					[335]
C_5H_7NS*		2,4-dimethylthiazole					
	222.9	2.90		13.0	51.7	2.9	11.5
		$A14+2*A15+2*A19+A18*B18+2A1+A131+A118$					[61]
$C_5H_8N_2O_2$		3-methyl-2,5-piperazinedione					
	543.9	30.62		56.3	52.8	30.6	28.7
		$A14+3*A15+2*A124+A16+A1$					[375]
C_5H_8O*		cyclopentanone					
	221.2	11.4		51.3	39.4	11.4	8.7
		$A14+2*A15+A114$					[393]
$C_5H_{10}N_2O_2$		N-acetylsarcosinamide					
	412.7	27.4	0	66.4	59.0	27.4	24.2
		$2*A1+A2+A59+A61$					[354]
$C_5H_{11}Br$		3-bromopentane					
	167.3	8.40		50.2	57.1	8.4	9.6
		$2*A1+2*A2+A3*B3+A21$					[312]
$C_5H_{12}O$		2-pentanol					
	200.0	8.48		42.4	41.3	8.5	8.3
		$2*A1+2*A2+A3*B3+A30$					[361]
$C_5H_{12}O$		3-pentanol					
	204.2	9.08		44.47	41.3	9.1	8.4
		$2*A1+2*A2+A3*B3+A30$					[361]
$C_6H_3ClN_2O_4$		2,4-dinitrochlorobenzene					
	325.2	20.2		62.0	51.3	20.2	16.7
		$3*A10+3*A12+2*A50+A22*C22$					[334]
$C_6H_3ClN_2O_4$		2,6-dinitrochlorobenzene					
	361.2	18.95		52.5	51.3	19.0	18.5
		$3*A10+3*A12+2*A50+A22*C22$					[334]
$C_6H_5ClO_3S$		4-chlorobenzene sulfonic acid					
	333.2	10.6		31.8	31.8	10.6	10.6
		$4*A10+2*A12+A22*B22+A145$					[348]
C_6H_6		2,4-hexadiyne					
	117.8	1.00		8.48	24	1.00	2.8
		$2*A1+4*A9$					[152]
$C_6H_7NO_2$		ethyl-α-cyanoacrylate					
	243.2	12.86		52.9	56.7	12.9	13.8
		$A1+A2+A5+A7+A38+A56$					[350]
$C_6H_8N_2O_2S$		*p*-aminobenzene sulfonamide					
	407.0	1.63	4.0				
	439.3	24.0	54.7	58.7	64.4	25.7	28.3
	438.7	23.0	52.4	56.4	64.4	24.7	28.3
		$4*A10+2*A12+A45+A96$					[305,395]
$C_6H_8O_4$		1,6-anhydro-2-deoxy-β-D-arabino-hexopyranose					
	323	12.55		38.9	56.9	12.6	18.4
		$2*A14+2*A15+4*A16+2*A30*D30+2*A112$					[376]
$C_6H_8O_6$*		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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
	466.15	37.04		79.5	84.2	79.5	39.2
		$A14+2*A15+4*A30*E30+2*A19+A16+A3*B3+A2+A115$					[392]
C_6H_9NO		N-vinylpyrrolidone					
	286.2	15.28		53.4	40.4	15.3	11.6
		$A14+2*A15+A6*B6+A5+A114+A119$					[368]
$C_6H_{10}B_2N_4$*		pyrazabole					
	354.3	11.83		33.4		11.8	
		Group value unavailable					[123]
$C_6H_{10}N_2O_2$		3,6-dimethyl-2,5-piperazinedione					
	556.1	30.6		55.1	55.7	30.6	31.0
		$A14+3*A15+2*A124+2*A16+2*A1$					[375]
$C_6H_{10}N_2O_2$		1,4-dimethyl-2,5-piperazinedione					
	418.2	22.0		52.7	36.3	22.0	15.2
		$A14+3*A15+2*A125+2*A1$					[375]
$C_6H_{10}O$*		cyclohexanone					
	221	8.51	38.5				
	242.6	1.25	5.2	43.7	43.1	9.8	10.5
		$A14+3*A15+A114$					[393]
$C_6H_{10}O_5$		1,6-anhydro-β-D-glucopyranose					
	385	24.9		64.8	59.4	24.9	22.9
		$2*A14+2*A15+5*A16+3*A30*E30+2*A112$					[376]
$C_6H_{10}O_5$		1,6-anhydro-β-D-glucopyranose					
	404	24.5		60.6	59.4	24.5	24.0
		$2*A14+2*A15+5*A16+3*A30*E30+2*A112$					[376]
$C_6H_{10}O_5$		1,6-anhydro-β-D-galactopyranose					
	401	22.8		56.9	59.4	22.8	23.8
		$2*A14+2*A15+5*A16+3*A30*E30+2*A112$					[376]
$C_6H_{10}O_5$		1,6-anhydro-β-D-altropyranose					
	375	2.43	6.5				
	388	18.0	46.4	52.8	59.4	23.1	20.4
		$2*A14+2*A15+5*A16+3*A30*E30+2*A112$					[376]
$C_6H_{10}O_5$		1,6-anhydro-β-D-mannopyranose					
	364	18.3		50.2	59.4	18.3	21.6
		$2*A14+2*A15+5*A16+3*A30*E30+2*A112$					[376]
$C_6H_{11}Cl$		1-chloro-1-methylcyclopentane					
	164.2	1.3	7.8				
	178.8	5.7	31.9				
	189.1	0.7	3.9	43.6	46.2	8.74	7.7
		$A14+A15*2+A1+A4*B4+A22$					[377]
$C_6H_{11}FO_5$		2-deoxy-2-fluoro-D-glucopyranose					
	427.2	38.2		89.4	79.0	38.2	33.8
		$A14+3*A15+A2+A112+4*A30*E30+5*A16+A28$					[336]
$C_6H_{11}FO_5$		3-deoxy-3-fluoro-D-glucopyranose					
	378.2	18.3		48.4	79.0	18.3	29.9
		$A14+3*A15+A2+A112+4*A30*E30+5*A16+A28$					[336]
$C_6H_{11}FO_5$		6-deoxy-6-fluoro-D-glucopyranose					
	412.2	27.2		66.0	74.3	27.2	30.6
		$A14+3*A15+A2+A112+4*A30*E30+5*A16+A27$					[336]
$C_6H_{11}NO_2$*		5,5-dimethylperhydro-1,3-oxazine-2-one					
	440.1	28.50		64.8	64.8	28.5	28.5
		$2*A1+A14+3*A15+A17+A125$					[297]
C_6H_{12}		4-methylpent-1-ene					
	118.9	4.93		41.5	48.5	4.9	5.8
		$2*A1+A2+A3+A5+A6$					[326]
$C_6H_{12}O_5$		1-deoxy-D-glucopyranose					
	403.2	27.4		68.0	76.3	27.4	30.8
		$A14+3*A15+A2+A112+4*A30*E30+4*A16$					[336]
$C_6H_{12}O_5$		2-deoxy-D-glucopyranose					
	398.7	34.5		86.5	76.3	34.5	30.4
		$A14+3*A15+A2+A112+4*A30*E30+4*A16$					[336]
$C_6H_{12}O_5$		3-deoxy-D-glucopyranose					
	387.2	32.6		84.2	76.3	32.6	29.5
		$A14+3*A15+A2+A112+4*A30*E30+4*A16$					[336]
$C_6H_{12}O_5$		6-deoxy-D-glucopyranose					

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

	T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	409.2	22.7		55.5	72.1	22.7	29.6
		A14+3*A15+A1+A112+4*A30*E30+5*A16					[336]
$C_6H_{12}O_6$		α-D-glucopyranose (α-D-glucose)					
	423.2	34.3		81.1	90.3	34.3	39.2
		A14+3*A15+5*A30*F30+A2+5*A16+A112					[336]
$C_6H_{12}O_6$		D-mannopyranose					
	391.2	24.7		63.1	90.3	24.7	35.3
		A14+3*A15+5*A30*F30+A2+5*A16+A112					[378]
$C_6H_{12}Si$		1-trimethylsilyl-1-propyne					
	204.5	10.96		53.6	37.7	11.0	7.7
		4*A1+A9+A109					[208,309]
$C_6H_{14}O_6$		L-iditol					
	352.8	30.90		87.6	108.0	30.9	38.1
		2*A2+4*A3*B3+6*A30*F30					[325]
$C_6H_{15}AsO_2$*		dipropylarsinic acid					
	408	22.1		54	39.6	16.2	22.1
		2*A1+4*A2+A142					[381]
$C_7H_5F_4NO_2$		1,1,3-trihydrotetrafluoropropyl α-cyanoacrylate					
	154.0	0.30	2.04				
	287.4	19.95	69.4	71.5	71.9	20.3	20.7
		A5+A7+A56+A38+A2+4*A26+A3*B3+A4*B4					[337]
$C_7H_5N_3O_6$		2,4,6-trinitrotoluene					
	352.2	23.4		66.5	53.4	23.4	18.8
		A1+3*A50+3*A12+A11+2*A10					[217]
$C_7H_8O_2$		4-methoxyphenol					
	328.4	18.30		55.7	57.2	18.3	18.8
		4*A10+2*A12+A1+A31+A32					[301]
$C_7H_{10}N_2O_2$		1,3,5-trimethyluracil					
	428.7	16.1		37.6	38.5	16.1	16.5
		A14+A15*3+2*A125+3*A1+A18*B18+A19					[379]
$C_7H_{12}N_2O_2$		N-acetyl-L-prolinamide					
	417.5	29.3		70.3	66.3	29.3	27.7
		A14+3*A15+A61+A16+A1+A146					[380]
$C_7H_{12}O$*		cycloheptanone					
	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
		A14+3*A15+A114					[393]
$C_7H_{14}N_2O_2$		N-acetyl-L-valinamide					
	509	39.1		76.8	56.0	39.1	28.5
		3*A1+A3*B3+A3+A61+A60					[380]
$C_7H_{14}O$		2-heptanone					
	237.7	19.71		82.9	77.0	19.7	18.3
		2*A1+4*A2*B2+A35					[214]
$C_7H_{14}O$		3-heptanone					
	236.0	17.53		74.3	74.8	17.5	17.7
		2*A1+3*A2*B2+A2+A35					[214]
$C_7H_{14}O$		4-heptanone					
	240.2	16.16		67.3	68.2	16.2	16.4
		2*A1+4*A2+A35					[214]
$C_7H_{14}O_6$		1-methoxy-α-D-glucopyranoside					
	424.2	37.6		88.6	83.9	37.6	35.6
		A14+3*A15+A1+A2+A32+A112+4*A30*E30+5*A16					[336]
$C_7H_{14}O_6$		3-methoxy-α-D-glucopyranoside					
	425.6	41.3		97.0	83.9	41.3	35.7
		A14+3*A15+A1+A2+A32+A112+4*A30*E30+5*A16					[336]
$C_7H_{14}O_6$		methyl α-D-mannopyranoside					
	455.2	44.7		98.2	83.9	44.7	38.2
		A14+3*A15+A1+A2+A32+A112+4*A30*E30+5*A16					[336]
$C_7H_{15}Br$		1-bromoheptane					
	214.4	21.76		101.5	90.9	21.8	19.5
		A1+6*A2*B2+A21					[333]
C_8BrF_{17}		1-bromoperfluorooctane					
	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)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_8H_5Br_3$		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]
$C_8H_8O_3$		5,6-dioxycarbony[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]
$C_8H_{10}O_4$		*trans, trans*-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]
$C_8H_{10}O_4$		*trans, cis*-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]
$C_8H_{12}B_2Cl_6O_5$*		1,3-diethyl-1,3-bis(trichloroacetoxy)-1,3-diboroxane					
	327.2	24.22		74.0		24.2	
		Group value unavailable					[186]
$C_8H_{12}N_2O_2$		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]
$C_8H_{14}O$*		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]
$C_8H_{16}B_2O_5$*		1,3-diacetoxy-1,3-diethyl-1,3-diboroxane					
	377.2	21.60		57.3		21.6	
		Group value unavailable					[186]
$C_8H_{16}N_2O_2$		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]
$C_8H_{16}N_2O_2$		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]
$C_8H_{16}O$*		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					
$C_8H_{16}O_4$*		12-crown-4					
	290.7	22.46		77.3	71.5	22.5	20.8
		A14+9*A15+4*A112					[398]
$C_8H_{17}Br$		1-bromooctane					
	218.2	24.69		113.2	100.2	24.7	21.9
		A1+7*A2*B2+A21					[333]
$C_8H_{18}O_4$		1,2,7,8-tetrahydroxyoctane					
	352.2	36.7		104.2	112.0	36.7	39.4
		4*A30*D30+6*A2+2*A3*B3					[346,347]
$C_8H_{18}Zn$*		di-*tert*-butyl zinc					
	300.0	45.30		151.0	70.8	45.3	21.2
		6*A1+2*A4*B4+A111					[294]
$C_8H_{18}AsO_2$*		dibutylarsinic acid					
	412	29.5		71.5	67.0	29.5	27.6
		2*A1+6*A2*B2+A142					[381]
$C_9H_8O_3$		*endo*-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]
$C_9H_8O_3$		*exo*-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]
$C_9H_8O_4$		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_{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)
$C_9H_{10}O_2$		2,3-dimethylbenzoic acid					
	417.6	18.30		43.8	44.1	18.3	18.4
		2*A1+3*A10+2*A11+A12+A36					[212]
$C_9H_{10}O_2$		3,5-dimethylbenzoic acid					
	442.9	22.60		51.0	44.1	22.6	19.5
		2*A1+3*A10+2*A11+A12+A36					[212]
$C_9H_{12}O$		2,6-diisopropylphenol					
	292.8	14.64		50.0	53.4	14.6	15.6
		4*A1+3*A10+2*A3+A31+2*A11+A12					[330]
$C_9H_{14}O$		bicyclo[3.3.1]nonan-9-one					
	300.5	14.11		47.0	47.1	14.1	14.1
		2*A14+3*A15+2*A16+A114					[159]
$C_9H_{14}N_2O_2$		1,3-dimethyl-5-propyluracil					
	355.0	26.3		74.2	52.7	26.3	18.7
		A14+3*A15+2*A125+3*A1+2*A2+A18*B18+A19					[379]
$C_9H_{14}N_2O_2$		1,3-dimethyl-5-isopropyluracil					
	354.7	22.4		63.0	39.7	22.4	14.1
		A14+3*A15+2*A125+4*A1+A3+A18*B18+A19					[379]
$C_9H_{15}N_3O_3$*		N-acetylglycyl-L-prolinamide					
	450.6	5.60	12.4				
	457.8	27.0	59.0	71.4	75.8	32.6	34.7
		A14+2*A15+A1+A2+A146+A61+A60+A35+A16					[355]
$C_9H_{15}N_3O_3$*		N-acetyl-L-prolyl-glycinamide					
	434.1	32.2		74.2	65.5	32.2	32.9
		A14+2*A15+A1+A2+A146+A61+A60+A35+A16					[356]
$C_9H_{16}O$*		cyclononanone					
	247	14.7	59.5				
	298	1.6	5.4	64.9	54.2	16.3	16.2
		A14+6*A15+A114					[393]
$C_9H_{19}Br$		1-bromononane					
	243.2	30.12		123.4	109.5	30.1	26.63
		A1+8*A2*B2+A21					[333]
$C_{10}H_{10}N_4O_2S$		sulfadiazine					
	538.7	31.2		58	78.8	31.2	42.5
		7*A10+3*A12+2*A41+A95+A45					[382]
$C_{10}H_{12}$		*exo*-dicyclopentadiene					
	189.8	7.11		37.5	48.3	7.1	9.2
		3*A14+A15+4*A18+4*A19					[339]
$C_{10}H_{12}$		*endo*-dicyclopentadiene					
	216.1	8.04	40.1				
	304.7	1.79	6.1	46.2	48.3	9.8	14.7
		3*A14+A15+4*A18+4*A19					[339]
$C_{10}H_{12}O_2$*		2-acetyl-3,5-dimethylphenol					
	333.2	1.36		4.08	61.4	1.4	20.5
		2*A12+2*A11+2*A10+3*A1+A31+A38					[11]
		Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					
$C_{10}H_{12}O_2$		acetophenone ethylene glycol ketal					
	333.6	25.2		75.5	53.6	25.2	17.9
		A14+2*A15+2*A112+A17+A1+5*A10+A11					[383]
$C_{10}H_{12}O_3$*		4-*n*-propoxybenzoic acid					
	394.2	7.95	20.17				
	419.7	16.74	39.89				
	426.7	2.51	5.88	65.9	67.3	27.2	28.7
		4*A10+2*A12+2*A2+A1+A36*B36+A32					
		Forms liquid crystal					[178]
$C_{10}H_{12}O_4$		2,5-diethoxy-1,4-benzoquinone					
	459.3	28.7		62.5	69.8	28.7	32.0
		2*A1+2*A2+A14+3*A15+2*A18+2*A19+2*A32+2*A114					[342]
$C_{10}H_{14}O$		L-carvone					
	247.7	11.55		46.6	54.8	11.6	13.6
		2*A1+A5+A7+A16+A18*B18+A19+A14+3*A15+A114					[211]
$C_{10}H_{15}F$*		1-fluoroadamantane					
	221.6	1.50		6.77	37.9	1.50	8.4

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

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

	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)
		$A14+2*A15+2*A19+2*A19+8*A10+A134$					[327]
$C_{12}H_{10}N_2$		1-methyl-9H-pyrido[3,4-*b*]indole					
	509.9	27.20		53.3	57.1	27.2	29.1
		$A1+A14+2*A15+2*A9+2*A19+6*A10+A11+A121+A41$					[323]
$C_{12}H_{10}O_2$		α-naphthyl acetate					
	319.2	20.21		63.3	54.6	20.2	17.4
		$7*A10+3*A12+A1+A38$					[118]
$C_{12}H_{10}O_2$		β-naphthyl acetate					
	342.2	20.05		58.6	54.6	20.1	18.7
		$7*A10+3*A12+A1+A38$					[118]
$C_{12}H_{10}O_2S$		diphenyl sulfone					
	398.2	21.78		54.7	59.3	21.8	23.6
		$10*A10+2*12+A88$					[327]
$C_{12}H_{10}S$		diphenylsulfide					
	258.0	13.98		54.19	61.10	13.98	15.76
		$10*A10+2*A12+84$					[207]
$C_{12}H_{10}Te$*		diphenyl telluride					
	268.4	15.35		57.2	57.0	15.4	15.3
		$10*A10+2*A12+A140$					[300]
$C_{12}H_{12}N_2$		benzidine					
	400.2	19.10		47.7	72.0	19.1	28.8
		$4*A12+8*A10+2*A45$					[4]
$C_{12}H_{14}N_4O_2S$		4-amino-N-[2,6-dimethyl-4-pyrimidinyl)benzene sulfonamide					
	515.6	45.11		87.5	58.6	45.1	30.2
		$2*A1+5*A10+3*A12+2*A11+2*A41+A95$					[358]
$C_{12}H_{14}N_4O_2S$		sulfisomidine					
	523.6	42.7		81.5	80.0	42.7	41.9
		$5*A10+2*A41+A95+A45+3*A12+2*A11+2*A1$					[382]
$C_{12}H_{14}N_4O_2S$		sulfamethazine					
	471.6	31.1		66.0	80.0	31.1	37.7
		$5*A10+3*A12+2*A11+2*A1+2*A41+A95+A45$					[382]
$C_{12}H_{16}O_2$*		4-*n*-pentylbenzoic acid					
	252.0	2.60	10.32				
	362.0	9.90	27.35				
	395.0	1.50	3.80	41.47	57.7	14.0	22.8
		$A1+2*A2+4*A10+A11+A12+A36$					[177]
		Forms liquid crystal					
$C_{12}H_{16}O_3$*		4-*n*-pentoxybenzoic acid					
	398.2	21.8	54.7				
	422.2	2.1	5.0	59.7	81.5	23.9	34.4
		$4*A10+2*A12+4*A2+A1+A36*B36+A32$					[178]
		Forms liquid crystal					
$C_{12}H_{16}O_4$		2,5-dipropoxy-1,4-benzoquinone					
	357.0	8.60	24.09				
	460.8	33.6	72.92	97.0	84.0	42.2	38.7
		$2*A1+4*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114$					[342]
$C_{12}H_{16}O_6$		α-phenoxy-α-D-glucopyranoside					
	429.2	39.0		90.9	95.8	39.0	41.1
		$A14+3*A15+A2+A32+A112+4*A30*E30+5*A16+5*A10+A12$					[384]
$C_{12}H_{18}N_2O_3S$*		3-(*p*-tolyl-4-sulfonyl)-1-butyl urea					
	404.8	25.6		63.3		25.6	
		Group value not available					[358]
$C_{12}H_{18}O$		2-(1′-cyclohexenyl)cyclohexanone					
	278.8	17.26		61.9	59.0	17.3	16.5
		$2*A14+6*A15+A18+A19+A16+A114$					[314]
$C_{12}H_{18}O$		3,5-diisopropylphenol					
	326.3	12.13		37.2	53.4	12.1	17.4
		$4*A1+3*A10+2*A3+A31+2*A11+A12$					[330]
$C_{12}H_{18}O_6$		R,R,R-4,8,12-trimethyl-1,5,9-trioxacyclododeca-2,6,10-trione					
	380.2	21.5		56.6	84.7	21.5	32.2
		$3*A1+A14+9*A15+3*A115+3*A16$					[206]
$C_{12}H_{20}O$		2-cyclohexylcyclohexanone					
	277.0	18.00		65.0	58.2	18.0	16.1
		$2*A14+6*A15+2*A16+A114$					[314]
$C_{12}H_{22}O$		cyclododecanone					
	335.6	16.85		50.2	65.3	16.9	21.9
	336.3	16.6		50		16.6	
		$A14+A114+9*A15$					[298,393]
$C_{12}H_{22}O$		*trans*-2-cyclohexylcyclohexanol					

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

	T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
	325.8	14.52		44.6	46.6	14.5	15.2
		2*A14+6*A15+3*A16+A30					[313]
$C_{12}H_{31}AsO_2$*		dihexylarsinic acid					
	393	16.4	41.8				
	405	24.35	60.1	101.9	104.2	40.7	42.2
		2*A1+10*A2*B2+A142					[381]
$C_{12}H_{36}O_6Si_6$		dodecamethylcyclohexasiloxane					
	269.0	28.58		106.3	76.9	28.6	20.7
		12*A1+6*A112+6*A139+A14+9*A15					[121]
$C_{13}H_8O_2$		S-(+)-4-isobutyl-α-methylphenyl acetic acid					
	325.5	18.70		57.5	57.5	18.7	18.7
		3*A1+A2+A3+A3*B3+4*A10+2*A11+A36					[319]
$C_{13}H_{10}N_2O_2$*		N-phenyl 4-nitrobenzaldehyde imine					
	347.15	24.56		70.7	64.0	24.6	22.2
		9*A10+3*A12+A6*B6+A42+A50					[397]
$C_{13}H_{10}O_2$*		(2-hydroxyphenyl)phenylmethanone					
	308.2	0.67		2.17		0.67	
		No prediction made: Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					[11]
$C_{13}H_{11}N$*		N-phenylbenzaldehyde imine					
	329.65	20.42		61.9	61.2	20.4	20.2
		10*A10+2*A12+A6*B6+A42					[397]
$C_{13}H_{12}N_2O$*		7-methoxy-1-methyl-9H-pyrido[3,4-*b*]indole					
	536.6	48.80		90.9	64.5	48.8	42.6
		2*A1+A14+2*A15+2*A19+2*A19+5*A10+A11+A121+A41+A32					[323]
$C_{13}H_{17}N_3O$*		aminopyrine					
	380	27.17		71.5	52.9	27.2	20.1
		A14+2*A15+4*A1+A43+A119+A125+5*A10+A12+2*A19					
$C_{13}H_{18}O_2$*		4-*n*-hexylbenzoic acid					
	371.0	17.40	46.90				
	380.0	2.40	6.31	53.21	65.1	19.80	24.7
		A1+2*A2+5*A10+A11+A12+A36					[177]
		Forms liquid crystal					
$C_{13}H_{18}O_2$		benzaldehyde 2,2-dimethylpropylene glycol acetal					
	307.6	18.6		60.5	60.2	18.6	18.5
		5*A10+A11+A14+3*A15+A17+A16+2*A1+2*A112					[385]
$C_{14}H_5F_{25}$*		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-pentacosofluorotetradecane					
	344.2	20.80		60.43	149.5	20.80	51.5
		12*A4*B4+3*A25+22*A26+A1+A2					[68]
		Amphiphillic compound					
$C_{14}H_9F_{17}O_2$*		perfluorooctylethylene methacrylate					
	210	5.0	23.8				
	253	9.0	35.6	59.4		14.0	
		Amphiphillic compound					[16]
$C_{14}H_9F_{21}O$*		ω-perfluorodecyl-1-butanol					
	360	21.30		59.2		21.3	
		Amphiphillic compound					[17]
$C_{14}H_{12}N_2O_2$		4-nitro-4′-methylbenzylidene aniline					
	402.0	27.30		67.9	64.6	27.3	25.9
		A1+8*A10+A11+3*A12+A42+A6*B6+A50					[302]
$C_{14}H_{12}O_2$*		(2-methoxyphenyl)phenylmethanone					
	350.2	0.68		1.94		0.7	
		No prediction made: Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					[11]
$C_{14}H_{14}O_3$*		Naproxen					
	428.5	31.5		73.5	58.6	31.5	25.1
		2*A1+A3*B3+6*A10+A11+2*A12+A32+A36*B36					[394]
$C_{14}H_{20}O_4$		2,5-dibutoxy-1,4-benzoquinone					
	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
		2*A1+6*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114					[342]
$C_{14}H_{22}$		1,4-di-*tert*-butylbenzene					
	341.5	22.48		65.8	46.4	22.5	15.9
		6*A1+4*A10+2*A11+2*A4					[362]
$C_{14}H_{23}NO_2$		*n*-decyl-α-cyanoacrylate					
	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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{14}H_{28}$		*trans*-1,4-di-*tert*-butylcyclohexane					
	363.2	17.15		47.2	51.1	17.2	18.6
		6*A1+A14+2*A15+2*A4+2*A16					[41]
$C_{14}H_{28}$		*cis*-1,4-di-*tert*-butylcyclohexane					
	293.2	8.79		30.0	51.1	8.8	15.0
		6*A1+A14+2*A15+2*A4+2*A16					[41]
$C_{14}H_{26}B_2N_4$*		4,4,8,8-tetraethylpyrazabole					
	342.4	28.61	83.61				
	379.2	3.22	8.49	92.1		31.8	
		Group value unavailable					[123]
$C_{14}H_{31}AsO_2$*		diheptylarsinic acid					
	299.0	30.1	100.7				
	389.0	20.3	52.3	153.0	122.8	50.4	47.7
		2*A1+12*A2*B2+A142					[381]
$C_{14}H_{42}O_7Si_7$		tetradecamethylcycloheptasiloxane					
	237.7	20.88		87.8	86.0	20.9	20.4
		14*A1+7*A112+7*A139+A14+11*A15					[121]
$C_{15}H_{11}NO_2$		1-(methylamino)-9,10-anthracenedione					
	443.2	28.81		65.0	49.1	28.8	21.8
		A14+3*A15+2*A114+4*A19+7*A10+A1+A44+A12					[315]
$C_{15}H_{12}ClN_5O_4$		5-[(4-chloro-2-nitrophenylazo]-1-ethyl-1,2-dihydro-6-hydroxy-4-methyl-2-oxo-3-pyridinecarbonitrile					
	500.2	35.16		70.3	85.8	35.2	42.9
		3*A10+3*A12+A50+A22*F22+2*A42+A30*F30+2*A1+A2+A56 +A14+3*A15+A125+4*A19					[315]
$C_{15}H_{12}N_2O_2$		5,5-diphenylhydantoin					
	574.0	36.29		63.2	66.4	36.3	38.1
		A14+2*A15+2*A124+A17+10*A10+2*A11					[395]
$C_{15}H_{14}O_2$*		(2-hydroxy-4,6-dimethylphenyl)phenylmethanone					
	405.2	0.67		1.65		0.67	
		No prediction made: Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					[11]
$C_{15}H_{16}S_2$		2,2-bis(phenylthio)propane					
	329.0	24.4		74.2	75.4	24.4	24.8
		2*A1+10*A10+2*A12+A4*B4+2*A84					[363]
$C_{15}H_{20}N_2O_4S$*		4-acetyl-N-[(cyclohexylamino)carbonyl]benzene sulfonamide					
	457.0	41.08		89.9		41.1	
		Group value not available					[358]
$C_{15}H_{21}NO_2$		1-methyl-4-phenylpiperidine-4-carboxylic acid ethyl ester (meperidine)					
	308.2	24.60		79.8	68.0	24.6	21.0
		2*A1+5*A10+A11+A38+A14+3*A15+A2+A17+A119					[296]
$C_{16}H_9F_{25}$*		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-pentacosafluorohexadecane					
	147	0.70	4.76				
	314	1.40	4.46				
	349	21.0	60.17	69.39	163.7	23.1	57.2
		3*A2+A1+12*A4*B4+3*A25+22*A26					[17]
		Amphiphillic compound					
$C_{16}H_{14}O_3$		(±)α-(3-benzoylphenyl)propionic acid					
	367.4	28.23		76.8	70.6	28.2	25.9
		9*A10+A11+2*A12+A35+A36*B36+A1+A3*B3					[209]
$C_{16}H_{16}$		2,2-metacyclophane					
	404.0	21.42		53.0	51.3	21.4	20.7
		A14+7*A15+4*A19+2*A18+6*A10					[316]
$C_{16}H_{16}$		2,2-metaparacyclophane					
	315.0	0.98	3.11				
	354.0	12.76	36.05	39.2	46.0	13.7	16.3
		A14+8*A15+4*A19+3A18+5*A10					[316]
$C_{16}H_{16}$*		2,2-paracyclophane					
	323.2	0.21		0.65	40.7	0.2	13.2
		A14+9*A15+4*A19+4*A18+4*A10					[360]
$C_{16}H_{16}O_2$*		(2-hydroxyphenyl)-2,4,6-trimethylphenylmethanone					
	353.2	0.49		1.39		0.49	
		No prediction made. Reported enthalpy of fusion is too small, and the published enthalpy and entropy of fusion data are internally inconsistent					[11]
$C_{16}H_{17}ClN_4O_4$*		2,2′-[[3-chloro-4-[(4-nitrophenyl)azo]phenyl]imino]bis-ethanol					
	463.2	29.78		64.3		29.8	
		Group value not available					[13]

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

	T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{16}H_{17}Cl_2N_5O_4$*		1-[[2-chloro-4-[(2-chloro-4-nitrophenyl)azo]-5-(methylamino)phenyl]amino]-2-propanol N-oxide					
	371.2	30.62		82.5	82.5	30.6	30.6
		Group value not available					[315]
$C_{16}H_{17}F_{15}O$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7-pentadecafluoro-8-hexadecanone					
	285.8	34.20		119.7	147.5	34.2	42.2
		7*A4*B4+3*A25+12*A26+A1+7*A2+A35					[23]
		Amphiphillic compound					
$C_{16}H_{20}O_3$		3-benzoyl-1,2,2-trimethylcyclopentanecarboxylic acid					
	387.6	20.35		52.5	60.0	20.4	23.3
		3*A1+A14+2*A15+2*A17+A16+2*A10+A12+A36*B36+A35					[366]
$C_{16}H_{23}N$*		N-cyclohexyl(2,4,6-trimethyl)benzaldehyde imine					
	339.4	25.61		75.5	92.1	25.6	31.2
		A14+3*A15+A16+3*A1+2*A10+A6*B6+A42+A12					[397]
$C_{16}H_{24}O_4$		2,5-dipentoxy-1,4-benzoquinone					
	333.7	9.0	26.97				
	414.6	36.5	88.04	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]
$C_{16}H_{35}AsO_2$*		dioctylarsinic acid					
	379	20.7	54.6				
	402	35.8	89	143.6	141.4	56.5	56.6
		2*A1+14*A2*B2+A142					[381]
$C_{17}H_{16}ClN_5O_3$		3-[[4-[(2-chloro-4-nitrophenyl)azo]phenyl](2-hydroxyethyl)amino]propanenitrile					
	428.2	26.29		61.4	90.7	26.3	38.8
		4*A2+7*A10+5*A12+A30*F30+A22*F22+A50+A56+2*A42+A43					[315]
$C_{17}H_{17}ClO_6$*		([2S]-*trans*-7-chloro-,2′,4,6-trimethoxy-6′-methylspiro[benzofuran-2(3H),1′-(2)cyclohexene]-3,4′-dione					
	495.2	39.39		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]
$C_{17}H_{17}Cl_2N_5O_4$		N-[4-chloro-2-[(2-chloro-4-nitrophenyl)azo]-5-[(2-hydroxypropyl)amino]phenyl] acetamide					
	471.2	38.87		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]
$C_{17}H_{19}NO_3$		7,8-didehydro-4-5-epoxy-17-methylmorphinan-3,6-diol (morphine)					
	528.2	28.87		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]
$C_{17}H_{19}NO_3$		4,5-epoxy-3-hydroxy-17-methylmorphinan-6-one (hydromorphone)					
	539.2	35.61		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]
$C_{17}H_{21}ClO_4$		3-(3-chloro-4-methoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	440.2	29.10		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]
$C_{17}H_{21}F_{15}$*		1,1,1,2,3,3,4,4,5,5,6,6-dodecafluoro-2-(trifluoromethyl)hexadecane					
	220.0	3.00	13.64				
	261.0	18.00	68.96	82.6	143.8	21.0	37.5
		7*A4*B4+6*A25+A27+8*A26+A1+9*A2					[22]
		Amphiphillic compound					
$C_{17}H_{21}NO_6$		3-(3-nitro-4-methoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	426.9	32.36		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]
$C_{17}H_{21}N_3O_2$		2,2′-[[3-methyl-4-4(phenylazo)phenyl]imino]bis-ethanol					
	384.2	31.90		83.0	88.4	31.9	34.0
		8*A10+3*A12+A11+2*A42+A1+4*A2+2*A30*E30+A43					[13]
$C_{17}H_{22}O_3$		3-(4-methylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	468.2	30.07		64.2	60.6	30.1	28.4
		4*A1+A14+2*A15+2*A17+A16+4*A10+A11+A12+A36*B36+A35					[372]
$C_{17}H_{23}NO_3$*		3-[(hydroxyimino)phenylmethyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
	422.0	33.80		80.1	67.4	33.8	28.4
		4*A1+A14+2*A15+A12+5*A10+2*A17+A7+A53+A38+A16					[373]
$C_{17}H_{23}NO_4$*		3-(4-methoxy-3-aminobenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	498.6	41.32		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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{18}HF_{15}Ge$*	tris(pentafluorophenyl)germane					
405.0	34.90		86.2	86.2	34.9	34.9
	18*A12+15*A24+A141					[308]
$C_{18}H_{11}NO_3$	2-(3-hydroxy-2-quinolinyl)-1H-indene-1,3(2H)-dione					
539.2	30.89		57.3	80.3	30.9	43.3
	9*A10+4*A12+A14+2*A15+4*A19+A114+A30*D30+A41					[315]
$C_{18}H_{13}F_{25}$*	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-pentacosofluorooctadecane					
317.2	3.30	10.4				
352.2	21.80	61.70	72.10	177.9	25.10	62.7
	12*A4*B4+3*A25+22*A26+A1+5*A2					[68]
	Amphiphillic compound					
$C_{18}H_{20}$	6-(4-biphenyl)-1-hexene					
274.5	15.10		55.0	93.0	15.1	25.5
	9*A10+2*A12+A11+4*A2+A5+A6					[97]
$C_{18}H_{20}$	3,3-paracyclophane					
332.0	7.36	22.17				
351.0	0.46	1.31				
377.0	11.76	31.19	54.7	48.1	19.6	18.1
	A14+11*A15+4*A19+4*A18+4*A10					[316]
$C_{18}H_{20}O_2$*	(2-hydroxyl-4,6-dimethylphenyl)-2,4,6-trimethylphenylmethanone					
380.2	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]
$C_{18}H_{21}N$*	N-benzyl-pivalophenone imine					
339.6	27.86		82.05	84.2	27.9	28.6
	10*A10+A11+A12+3*A1+A4+A2+A6*B6+A42					[397]
$C_{18}H_{21}NO_3$	7,8-didehydro-4,-5-epoxy-3-methoxy-17-ethylmorphanan-6-ol (codeine)					
430.3	23.81		55.3	62.6	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]
$C_{18}H_{22}O_4$	4,4′-di-(2-methoxyethoxy)biphenyl					
409.5	17.53	42.81				
412.4	22.67	54.97	97.8	111.6	40.2	40.3
	2*A1+4*A2+8*A10+4*A12+4*A32					[345]
$C_{18}H_{24}N_2O_6$*	3-[(hydroxyimino)(4-methoxy-3-nitrophenyl)methyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
433.0	31.99		73.9	77.6	32.0	33.6
	5*A1+A14+2*A15+3*A12+3*A10+2*A17+A16+A38+A32 +A50+A7+A53					[373]
$C_{18}H_{24}O_3$	3-(4-ethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
387.6	22.54		58.2	67.7	22.5	26.3
	4*A1+A14+2*A15+2*A17+A16+4*A10+A2+A11+A12+A36*B36+A35					[366]
$C_{18}H_{24}O_3$	3-(3,4-dimethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
460.6	32.31		70.2	61.2	32.3	28.2
	5*A1+A14+2*A15+2*A17+A16+3*A10+2*A11+A12+A36*B36+A35					[366]
$C_{18}H_{24}O_3$	3-(2,4-dimethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
386.8	18.81		48.6	61.2	18.8	23.7
	5*A1+A14+2*A15+2*A17+A16+3*A10+2*A11+A12+A36*B36+A35					[366]
$C_{18}H_{24}O_4$	3-(4-ethoxybenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
394.6	22.05		55.9	88.5	22.1	34.9
	4*A1+A14+2*A15+2*A17+A16+4*A10+A2+2*A12+A36*C36+A35+A32					[366]
$C_{18}H_{25}NO_3$	3-[4-(dimethylamino)benzoyl]-1,2,2-trimethylcyclopentanecarboxylic acid					
445.0	25.03		56.3	72.1	25.0	32.1
	5*A1+A14+2*A15+2*A17+A16+4*A10+2*A12+A36*C36+A35+A43					[366]
$C_{18}H_{25}NO_4$*	3-[(hydroxyimino)(4-methoxyphenyl)methyl]-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
433.0	36.99		85.4	74.8	37.0	32.4
	5*A1+A14+2*A15+2*A12+4*A10+2*A17+A16+A38+A32+A53+A7					[373]
$C_{18}H_{28}O_4$	2,5-di-*n*-hexyloxy-1,4-benzoquinone					
332.3	5.3	15.95				
412.1	38.9	94.39	110.3	126.6	44.2	52.2
	2*A1+10*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114					[342]
$C_{18}H_{32}O_2$	linoelaidic acid					
303	47.70		157.4	163.8	47.7	49.6
	A1+12*A2*B2+4*A6+A36					[331]
$C_{18}H_{32}O_2$	4-octadecynoic acid					

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

	T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
	348	57.94		166.5	151.2	57.9	52.6
		$A1+12*A2*B2+2*A9+A36+2*A2$					[331]
$C_{18}H_{32}O_2$		5-octadecynoic acid					
	325	54.41		167.4	149.0	54.4	48.4
		$A1+11*A2*B2+2*A9+A36+3*A2$					[331]
$C_{18}H_{32}O_2$		6-octadecynoic acid					
	324	54.92		169.5	155.6	54.9	50.4
		$A1+14*A2*B2+2*A9+A36$					[331]
$C_{18}H_{32}O_2$		7-octadecynoic acid					
	322	53.61		166.5	155.6	53.6	50.1
		$A1+14*A2*B2+2*A9+A36$					[331]
$C_{18}H_{32}O_2$		8-octadecynoic acid					
	320	55.30		172.8	155.6	55.3	49.8
		$A1+14*A2*B2+2*A9+A36$					[331]
$C_{18}H_{32}O_2$		9-octadecynoic acid					
	319	54.87		172.0	155.6	54.9	49.6
		$A1+14*A2*B2+2*A9+A36$					[331]
$C_{18}H_{32}O_2$		10-octadecynoic acid					
	319	52.23		164.0	155.6	52.3	49.6
		$A1+14*A2*B2+2*A9+A36$					[331]
$C_{18}H_{32}O_2$		11-octadecynoic acid					
	320	55.97		174.9	155.6	56.0	49.8
		$A1+14*A2*B2+2*A9+A36$					[331]
$C_{18}H_{32}O_2$		12-octadecynoic acid					
	320	49.79		155.6	155.6	49.8	49.8
		$A1+14*A2*B2+2*A9+A36$					[331]
$C_{18}H_{32}O_2$		13-octadecynoic acid					
	322	55.51		172.4	155.6	55.5	50.1
		$A1+14*A2*B2+2*A9+A36$					[331]
$C_{18}H_{32}O_2$		14-octadecynoic acid					
	337	52.74		156.5	151.2	52.7	51.0
		$A1+12*A2*B2+2*A9+A36+2*A2$					[331]
$C_{18}H_{32}O_2$		16-octadecynoic acid					
	347	60.10		173.2	155.6	60.1	54.0
		$A1+14*A2*B2+2*A9+A36$					[331]
$C_{18}H_{32}O_2$		17-octadecynoic acid					
	340	54.20		159.4	157.7	54.2	52.9
		$15*A2*B2+A9+A36+A8$					[331]
$C_{18}H_{34}B_4N_4$*		4,4,8,8-tetrapropylpyrazabole					
	382.2	33.00		86.3		33.0	
		Group value unavailable					[123]
$C_{18}H_{34}O_2$		*trans*-3-octadecenoic acid					
	334	57.15		171.1	169.6	57.2	56.7
		$A1+13*A2*B2+2*A6+A36+A2$					[331]
$C_{18}H_{34}O_2$		*trans*-4-octadecenoic acid					
	333	55.88		167.8	167.4	55.9	55.7
		$A1+12*A2*B2+2*A6+A36+2*A2$					[331]
$C_{18}H_{34}O_2$		*trans*-5-octadecenoic acid					
	319	45.11		141.3	165.2	45.1	52.7
		$A1+11*A2*B2+2*A6+A36+3*A2$					[331]
$C_{18}H_{34}O_2$		*trans*-6-octadecenoic acid					
	326	60.15		184.5	171.8	60.2	56.0
		$A1+14*A2*B2+2*A6+A36$					[331]
$C_{18}H_{34}O_2$		*trans*-10-octadecenoic acid					
	326	58.52		179.5	171.8	58.5	56.0
		$A1+14*A2*B2+2*A6+A36$					[331]
$C_{18}H_{34}O_2$		*trans*-11-octadecenoic acid					
	317	58.49		184.5	171.8	58.5	54.5
		$A1+14*A2*B2+2*A6+A36$					[331]
$C_{18}H_{34}O_2$		*trans*-12-octadecenoic acid					
	325	56.71		174.5	171.8	56.7	55.8
		$A1+14*A2*B2+2*A6+A36$					[331]
$C_{18}H_{34}O_2$		*trans*-13-octadecenoic acid					
	318	55.62		174.9	165.2	55.6	52.5
		$A1+11*A2*B2+2*A6+A36+3*A2$					[331]

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

	T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{18}H_{34}O_2$		*trans*-14-octadecenoic acid					
	327	57.06		174.5	167.4	57.1	54.7
		*A*1+12**A*2**B*2+2**A*6+*A*36+2**A*2					[331]
$C_{18}H_{34}O_2$		*trans*-15-octadecenoic acid					
	331	58.98		178.2	169.6	59.0	56.1
		*A*1+13**A*2**B*2+2**A*6+*A*36+*A*2					[331]
$C_{18}H_{36}$		*cis, cis*-1,3,5-tri-*tert*-butylcyclohexane					
	393.2	26.78		68.1	54.4	26.8	21.4
		9**A*1+*A*14+3**A*15+3**A*4+3**A*16					[41]
$C_{18}H_{36}$		*cis, trans*-1,3,5-tri-*tert*-butylcyclohexane					
	338.2	17.99		53.2	54.4	18.0	18.4
		9**A*1+*A*14+3**A*15+3**A*4+3**A*16					[41]
$C_{18}H_{38}O_2$		2-(hexadecyloxy)ethanol					
	311.7	14.94	47.93				
	318.5	37.32	117.2	165.1	193.7	52.3	61.7
		*A*1+15**A*2**B*2+*A*32+*A*30**B*30+2*A*2					[88]
$C_{18}H_{38}O_9$		1,ω-dimethoxyocta(oxyethylene)					
	276.2	60.1		217.6	226.4	60.1	62.5
		2**A*1+16**A*2**B*2+9**A*32					[386]
$C_{18}H_{39}AsO_2$		di-*n*-nonylarsinic acid					
	383	24.3	63.5				
	399	38.1	95.5	159	160	62.4	63.8
		2**A*1+16**A*2**B*2+*A*142					[381]
$C_{18}H_{54}O_9Si_9$		octadecamethylcyclononasiloxane					
	246.2	25.64		104.1	104.2	25.6	25.7
		18**A*12+9**A*139+9**A*112+*A*14+15**A*15					[121]
$C_{19}H_{21}F_{19}$*		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**A*4**B*4+6**A*25+*A*27+12**A*26+*A*1+9**A*2					[22]
		Amphiphillic compound					
$C_{19}H_{15}N$*		N-phenyl benzophenone imine					
	392.3	29.14		74.3	76.0	29.14	29.8
		15**A*10+3**A*12+*A*7+*A*42					[397]
$C_{19}H_{24}O_3$*		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**A*1+2**A*14+4**A*15+2**A*17+*A*16+2**A*19+3**A*10+*A*12+*A*36**B*36+*A*35					[366]
$C_{19}H_{26}O_4$		3-(4-methoxy-2,6-dimethylbenzoyl)-1,2,2-trimethylcyclopentanecarboxylic acid					
	416.7	28.31		67.9	82.6	28.3	34.4
		6**A*1+*A*14+2**A*15+2**A*17+*A*16+2**A*10+2**A*12+2**A*11+*A*36**C*36+*A*35+*A*32					[366]
$C_{19}H_{26}O_6$		1,2,2-trimethyl-3-(2,4,6-trimethoxybenzoyl)cyclopentanecarboxylic acid					
	432.2	29.68		68.7	96.2	29.7	41.6
		6**A*1+*A*14+2**A*15+2**A*17+*A*16+2**A*10+4**A*12+*A*36**E*36					[366]
		+*A*35+3**A*32					
$C_{19}H_{27}NO_3$*		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**A*1+*A*14+2**A*15+2**A*11+*A*12+3**A*10+2**A*17+*A*16+*A*38+*A*53+*A*7					[373]
$C_{19}H_{27}NO_4$*		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**A*1+*A*14+2**A*15+2**A*12+4**A*10+2**A*17+*A*16+*A*38+*A*32+*A*2+*A*7+*A*53					[373]
$C_{19}H_{27}NO_5$*		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**A*1+*A*14+2**A*15+3**A*12+3**A*10+2**A*17+*A*16+*A*38+2**A*32+*A*7+*A*53					[373]
$C_{19}H_{38}O_2$*		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**A*1+*A*2+15*A*2**B*2+*A*38					[391]
$C_{20}H_{13}NO_4$		1-amino-4-hydroxy-2-phenoxy-9,10-anthracenedione					
	458.2	30.79		67.2	82.9	30.8	38.0
		*A*14+3**A*15+10**A*10+4**A*12+*A*31+*A*45+*A*32+2**A*114+4**A*19					[315]
$C_{20}H_{17}F_{25}$*		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-pentacosafluoroeicosane					
	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

	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)
							[17]
	324.2	5.60	17.27				
	355.2	21.90	61.66	78.93	467.7	27.50	166.1
		12*A4*B4+3*A25+22*A26+A1+7*A2					[68]
		Amphiphillic compound (values represent two sets of independent measurements)					
$C_{20}H_{17}N_3O_4$*		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	
		No prediction made (reporting authors express concern that the enthalpy is too small)					[315]
$C_{20}H_{19}BrS$*		2-*n*-buty1-5-(4-bromobiphenyl-4-yl)thiophene					
	501.4	21.40		42.7	101.5	21.4	50.9
		A1+3*A2+8*A10+4*A12+A21+A14+2*A15+A131+2*A19+2*A18					[14]
$C_{20}H_{21}F_{21}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosafluoroeicosane					
	317	4.0	12.62				
	337	24.4	72.38	85.0	186.6	28.4	62.8
							[17]
	306.5	2.20	7.18				
	336.7	26.70	79.30	86.5	186.6	28.9	62.8
		10*A4*B4+3*A25+18*A26+A1+9*A2					[24]
		(Values represent two sets of independent measurements) Amphiphillic compound					
$C_{20}H_{21}F_{19}O$*		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					[21]
		Amphiphillic compound					
$C_{20}H_{23}F_{19}O$*		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				
	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					[23]
		Amphiphillic compound					
$C_{20}H_{24}$		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					[97]
$C_{20}H_{24}O_6$		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					[398]
$C_{20}H_{26}O_3$		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					[366]
$C_{20}H_{28}O_5$		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					[366]
$C_{20}H_{32}O_4$		2,5-di-*n*-heptyloxy-1,4-benzoquinone					
	275.8	3.6	13.05				
	372.5	17.3	46.44				
	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					[342]
$C_{20}H_{40}O_2$*		methyl nonadecanoate					
	304.2	19.4	63.7				
	313.2	42.8	136.8	200.5	189.5	62.2	56.6
		2*A1+17*A2*B2+A38					[391]
$C_{20}H_0O_4$		2,2,12,12-tetramethyl-1,3,11,13-tetraoxycycloeicosane					
	369.5	45.60		123.4	102.3	45.6	37.8
		4*A1+A14+17*A15+2*A17+4*A112					[47]
$C_{20}H_{42}O_{10}$		1,ω-dimethoxynona(oxyethylene)					
	289.2	73.9		255.6	249.7	73.9	62.5
		2*A1+18*A2*B2+10*A32					[386]
$C_{20}H_{43}AsO_2$*		di-*n*-decylarsinic acid					
	380	24.5	64.4				
	400	42.3	105.9	170.2	178.6	66.8	71.4
		2*A1+18*A2*B2+A142					[381]
$C_{20}H_{50}Si_5$		decaethylcyclopentasilane					
	254.8	16.3	63.97				
	440.1	1.40	3.18	67.2	114.3	17.7	50.3
		10*A1+10*A2+A14+2*A15+5*A139					[175]
$C_{20}H_{60}O_{10}Si_{10}$		eicosanomethylcyclodecasiloxane					
	265.8	39.76		149.6	113.3	39.8	30.1
		20*A1+10*A139+10*A112+A14+17*A15					[121]
$C_{21}H_{20}BrN_7O_6$		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)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
		4-methoxyphenyl] acetamide					
	465.2	59.08		127.0	99.7	59.1	46.4
		4*A10+8*A12+3*A2+2*A1+A5+A6+2*A50+A21+2*A42+A32+A60+A56+A43					[315]
$C_{21}H_{20}N_4O_3$*		4-methoxy-N,N-bis(3-pyridinylmethyl)-1,3-benzenedicarboxamide					
	403.9	28.43		70.4	101	28.4	40.8
		11*A10+2*A11+3*A12+2*A41+2*A2+2*A60+A1+A32					[392]
$C_{21}H_{25}F_{19}$*		1,1,1,2,3,3,4,4,5,5,6,6,7,7,8,8-hexadecafluoro-(trifluoromethyl)eicosane					
	310.1	34.00		109.6	177.7	34.0	55.1
		9*A4*B4+6*A25+A27+12*A26+A1+11*A2					[22]
$C_{21}H_{29}NO_3$*		3-[(hydroxyimino)(5,6,7,8-tetrahydro-2-naphthalenyl)methyl-1,2,2-trimethylcyclopentanecarboxylic acid methyl ester					
	425.0	38.37		90.3	72.5	38.4	30.8
		4*A1+2*A14+5*A15+3*A10+2*A19+2*A17+A12+A16+A38+A7+A53					[373]
$C_{21}H_{30}O$		1,1′-diadamantyl ketone					
	404.7	5.90	14.57				
	470.0	15.70	33.40	48.0	55.0	21.6	25.9
		6*A14+2*A15+6*A16+2*A17+A35					[324]
$C_{21}H_{40}$		*trans*-2-heptyl-6-butyldecalin					
	295.3	31.80		107.7	121.9	31.8	36.0
		2*A14+4*A15+4*A16+2*A1+9*A2					[40]
$C_{21}H_{40}$		*trans*-2-propyl-6-octyldecalin					
	308.8	41.00		133.0	121.9	41.0	37.6
		2*A14+4*A15+4*A16+2*A1+9*A2					[40]
$C_{21}H_{42}O_2$*		ethyl nonadecanoate					
	300.2	18.49	61.6				
	309.2	43.18	139.7	201.3	189.5	61.7	56.6
		2*A1+A2+17*A2*B2+A38					[391]
$C_{21}H_{42}O_2$*		methyl eicosanoate					
	319.2	73.7		231	210	73.7	61.7
		2*A1+18*A2*B2+A38					[391]
$C_{21}H_{43}NO$		N-propylstearamide					
	348.0	16.02	46.03				
	354.0	50.04	141.4	187.4	199.7	66.1	70.7
		2*A1+16*A2*B2+A60+2A2					[291]
$C_{21}H_{43}NO$		N-heptylmyristamide					
	316.0	6.54	20.70				
	343.0	49.02	142.9	163.6	204.1	55.6	70.0
		2*A1+18*A2*B2+A60					[291]
$C_{21}H_{43}NO$		N-decylundecanamide					
	337.0	0.07	0.21				
	344.0	42.45	123.4	123.6	204.1	42.5	70.2
		2*A1+18*A2*B2+A60					[291]
$C_{21}H_{43}NO$		N-laurylnonanamide					
	328.0	0.17	0.52				
	341.0	66.91	196.2	196.7	204.1	67.1	69.6
		2*A1+18*A2*B2+A60					[291]
$C_{21}H_{43}NO$		N-myristylheptanamide					
	313.0	2.08	6.65				
	334.0	52.68	157.7	164.4	204.1	54.8	68.2
		2*A1+18*A2*B2+A60					[291]
$C_{21}H_{43}NO$		N-stearylpropanamide					
	337.0	1.84	5.45				
	350.0	56.03	160.1	165.6	201.9	57.9	70.7
		2*A1+17*A2*B2+A60+A2					[291]
$C_{22}H_{21}F_{25}$*		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-pentacosafluorodocosane					
	207	1.0	4.83				
	342	9.5	27.78				
	365	25.8	70.68	103.3	206.3	36.3	75.3
							[17]
	339.2	7.50	22.11				
	357.2	22.20	62.15	84.26	206.3	29.7	73.7
		12*A4*B4+3*A25+22*A26+A1+9*A2					[68]
		Amphiphillic compound (values represent two sets of independent measurements)					
$C_{22}H_{24}O_3$*		3-([1,1-biphenyl]-4-ylcarbonyl)-1,2,2,-trimethylcyclopentanecarboxylic acid					
	444.2	27.69		62.3	74.6	27.7	33.1
		3*A1+A14+2*A15+2*A17+A16+9*A10+3*A12+A36*B36+A35					[366]
$C_{22}H_{25}F_{21}$*		1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosofluorodocosane					
	334.1	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

	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)
		10*A4*B4+18*A26+3*A25+A1+11*A2					[22]
		Amphiphillic compound					
$C_{22}H_{26}N_2O_2$		(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]
$C_{22}H_{26}N_2O_2$		(2R, 3R, 6R, 7R)-2,6-diphenyl-3,4,7,8-tetramethyl-cis-perhydro-[1,4]-oxazino-[3,2-*b*]-[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]
$C_{22}H_{28}N_2O$		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-*n*-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]
$C_{22}H_{30}N_2O_2S$		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-*n*-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-*n*-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]
$C_{23}H_{24}N_6O_4$		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]
$C_{23}H_{25}BrN_6O_{10}$		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-*n*-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-*n*-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]
$C_{23}H_{44}$		*trans*-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]
$C_{23}H_{44}$		*trans*-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]
$C_{24}H_{18}N_2S_2$*		4,4′-bis-(2-thienylmethylidenamino)-*trans*-stilbene					
	567.2	44.90	79.16				
	580.2	0.20	0.34	79.5		45.1	
		No prediction made (forms liquid crystal)					[86]
$C_{24}H_{18}N_2S_2$*		1,2-bis-[5-(β-azastyryl)-2-thienyl]-*trans*-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_{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)
	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						[22]
$C_{24}H_{25}F_{25}$*		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-pentacosofluoro-14-methyltricosane					
	220.0	9.00	34.61				
	347.1	25.00	72.02	106.6	207.5	34.0	72.0
	12*A4*B4+3*A25+22*A26+2*A1+A3+9*A2						
	Amphiphillic compound						[22]
$C_{24}H_{30}O_4$		2,2′-diphenyl-bi(5,5-dimethyl-1,3-dioxan-2-yl)					
	507.1	49.8		98.2	80.6	49.8	40.9
	2*A14+6*A15+4*A17+4*A112+10*A10+2*A11+4*A1						[385]
$C_{24}H_{32}$*		8-[4-(4′-*n*-butylbiphenyl)]-1-octene					
	248.6	2.20	8.85				
	315.6	9.60	30.4	39.3	129.1	11.8	40.7
	8*A10+2*A12+2*A11+A5+A6+A1+9*A2						[97]
	Forms liquid crystal						
$C_{24}H_{40}O_4$		2,5-di-*n*-nonyloxy-1,4-benzoquinone					
	352.6	8.0	22.69				
	383.8	24.2	63.05				
	402.7	47.1	117.0	202.7	169.2	79.3	68.1
	2*A1+16*A2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114						[342]
$C_{24}H_{40}O_8$		dibenzo[24-crown-8]					
	354.1	16.6	46.9				
	375.4	52.25	139.2	186.1	130.1	68.85	49.1
	A14+15*A15+6*A112+4*A19+8*A10						[398, 399]
$C_{24}H_{44}$		*trans*-2,6-diheptyldecalin					
	326.7	40.17		123.0	143.2	40.2	46.8
	2*A1+4*A15+4*A16+2*A1+11*A2						[40]
$C_{24}H_{44}O_2$		3,3,7,7,11,11,15,15-octamethylcyclohexadecane-1,9-dione					
	423.2	34.30		81.0	81.1	34.3	34.3
	8*A1+4*A17+2*A114+A14+13*A15						[115]
$C_{24}H_{50}O_2$*		2-(docosanoxy)ethanol					
	317.2	12.92	40.73				
	335.9	43.93	130.8	171.5	249.5	56.9	83.8
	A1+21*A2*B2+A32+A30*B30						[88]
$C_{24}H_{51}AsO_2$*		di-*n*-dodecylarsinic acid					
	385	31.4	81.5				
	398	49.4	124.1	205.7	215.8	80.8	85.9
	2*A1+22*A2*B2+A142						[381]
$C_{24}H_{72}O_{12}Si_{12}$		tetracosamethylcyclododecasiloxane					
	234.2	15.45		65.97	131.5	15.5	30.8
	24*A1+12*A139+12*A112+A14+21*A15						[121]
$C_{26}H_{22}N_2O_2S_2$*		1,2-bis-[5-(4-methoxy-β-azastyryl)-2-thienyl]-*trans*-ethylene					
	538.2	63.50	118.0				
	567.2	0.80	1.41	119.4	123.2	64.30	69.88
	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				[86]
$C_{26}H_{29}F_{25}$*		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-pentacosafluorohexacosane					
	363	16.3	44.90				
	366	26.1	71.31	116.2		42.4	
							[17]
	359.2	26.0	72.38			26.0	
	Amphiphillic compound (values represent two sets of independent measurements)						[68]
$C_{26}H_{42}O$*		*trans*-1-(4-heptanoylphenyl)-4-heptylcyclohexane					
	343.2	16.49	48.05				
	344.7	7.71	22.37	70.4	145.5	24.2	50.2
	A14+3*A15+2*A16+4*A10+A11+A12+2*A1+11*A2+A35						[25]
	Forms liquid crystal						
$C_{26}H_{48}O_2$		4,4,7,7,13,13,16,16-octamethylcyclooctadecane-1,10-dione					
	492.2	50.60		102.8	88.5	50.6	43.6
	8*A1+4*A17+2*A114+A14+15*A15						[115]
$C_{26}H_{54}O$		1-hexacosanol					
	332.2	16.74	50.39				
	351.7	67.78	192.7	243.1	251.8	84.5	88.6
	A1+25*A2*B2+A30						[78]

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

	T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
$C_{26}H_{55}AsO_2$*		di-*n*-tridecylarsinic acid					
	388	36.5	94.0				
	396	52.7	133.1	227.2	234.4	89.2	92.8
		2*A1+24*A2*B2+A142					[381]
$C_{27}H_{42}Cl_2N_2O_6$*		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]
$C_{28}H_{22}N_2O_2$		1,4-[bis[(4-methylphenyl)amino]-9,10-anthracenedione					
	491.2	36.59		74.5	71.5	36.6	35.1
		3*A15+A14+14*A10+4*A19+2*A114+4*A12+2*A1+2*A11+2*A44					[315]
$C_{28}H_{31}F_{25}$*		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
		12*A4*B4+3*A25+22*A26+A1+15*A2					[68]
		Amphiphillic compound					
$C_{28}H_{48}O$*		*trans*-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]
$C_{28}H_{48}O_4$		2,5-di-*n*-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
		2*A1+20*A2*B2+A14+3*A15+2*A18*B18+2*A19+2*A32+2*A114					[342]
$C_{28}H_{52}O_2$		4,4,8,8,14,14,18,18-octamethylcycloeicosane-1,11-dione					
	418.2	36.80		88.0	95.9	36.8	40.1
		8*A1+4*A17+2*A114*+A14+17*A15					[115]
$C_{28}H_{59}AsO_2$*		di-*n*-tetradecylarsinic acid					
	390	39.3	100.6				
	397	58.2	146.6	247.2	253.0	97.5	100.5
		2*A1+26*A2*B2+A142					[381]
$C_{29}H_{41}NO_4$		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]
$C_{30}H_{37}F_{25}$*		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
		12*A4*B4+3*A25+22*A26+A1+17*A2					[68]
$C_{30}H_{56}O_2$		5,5,8,8,16,16,19,19-octamethylcyclodocosane-1,12-dione					
	442.2	47.70		107.9	95.9	47.7	42.4
		8*A1+4*A17+2*A114+A14+17*A15					[115]
$C_{30}H_{60}O_{15}$		45-crown-15					
	311.2	70.6		227	206.8	70.6	64.3
		A14+42*A15+15*A112					[386]
$C_{30}H_{63}AsO_2$*		di-*n*-pentadecylarsinic acid					
	390	46.4	119				
	396	63.6	160.5	279.6	271.6	110.0	107.6
		2*A1+28*A2*B2+A142					[381]
$C_{31}H_{43}NO_5$		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
		6*A14+2*A15+6*A1+2*A4+A30*E30+4*A16+3*A17+A119+A112+ 3*A19+A12+2*A10+A2+A38					[320]
$C_{32}H_{34}$		1,8-bis-(4-biphenyl)octane					
	415.2	56.00		134.9	140.8	56.0	58.5
		18*A10+4*A12+2*A11+8*A2					[97]
$C_{32}H_{34}$*		1,8-bis[4(4′-ethylbiphenyl)]butane					
	454.2	46.00		101.3	127.8	46.0	58.1
		2*A1+6*A2+16*A10+4*A12+4*A11					[97]
$C_{32}H_{41}F_{25}$*		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
		12*A4*B4+3*A25+22*A26+A1+19*A2					[68]
$C_{32}H_{64}16$		48-crown-16					
	312.2	59.1		189.4	219.1	59.1	68.4
		A14+45*A15+16*A112					[386]

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

	T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}}H_{tpce}$ (expt)	$\Delta_0^{T_{fus}}H_{tpce}$ (calcd)
$C_{32}H_{45}NO_5$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-(1-oxopropoxy)-6,14-ethenomorphinan-7-methanol					
	410.2	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]
$C_{32}H_{60}O_2$		5,5,9,9,17,17,21,21-octamethylcyclotetracosane-1,13-dione					
	380.2	32.60		85.7	110.7	32.6	42.1
		8*A1+4*A17+2*A114+A14+21*A15					[115]
$C_{32}H_{67}AsO_2$*		di-*n*-hexadecylarsinic acid					
	389	47.4	121.9				
	395	66.8	169.2	291	290.2	114.2	114.6
		2*A1+30*A2*B2+A142					[381]
$C_{33}H_{47}NO_5$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-(1-oxobutoxy)-6,14-ethenomorphinan-7-methanol					
	422.1	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]
$C_{34}H_{31}ClN_2O_3$*		spiro[isobenzofuran-1(3H),9′(9H)-7′-chloro-6′-(methylcyclohexylamino)-3′-methyl-2′-anilinoxanthene]-3-one					
	442.2	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]
$C_{34}H_{32}N_2O_3$		spiro[isobenzofuran-1(3H),9′(9H)-6′-(methylcyclohexylamino)-3′-methyl-2′-anilinoxanthene]-3-one					
	476.2	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]
$C_{34}H_{38}$*		1,6-*bis*-[4-(4′-ethylbiphenyl)]hexane					
	393.2	3.90	9.92				
	422.2	35.00	82.90	92.83	142.0	38.9	60.0
		2*A1+8*A2+16*A10+4*A11+4*A12					[97]
$C_{34}H_{49}NO_5$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-(1-oxopentoxy)-6,14-ethenomorphinan-7-methanol					
	379.1	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]
$C_{34}H_{68}O_{17}$		51-crown-17					
	301.2	66.6		221.1	231.4	66.6	69.7
		A14+48*A15+17*A112					[386]
$C_{34}H_{71}AsO_2$*		di-*n*-octadecylarsinic acid					
	390	50.9	130.6				
	393	68.6	174.5	305.1	308.8	119.5	121.4
		2*A1+32*A2*B2+A142					[381]
$C_{35}H_{51}NO_5$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-(1-oxohexyloxy)-6,14-ethenomorphinan-7-methanol					
	352.6	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]
$C_{36}H_{42}$*		1,8-*bis*-[4-(4′-ethylbiphenyl)]octane					
	402.2	8.40	20.89				
	413.2	42.00	101.6	122.5	156.2	50.4	64.5
		2*A1+16*A10+4*A12+4*A11+10*A2					[97]
$C_{36}H_{42}$*		1,4-*bis*-[4-(4′-*n*-butylbiphenyl)]butane					
	404.2	12.00	29.68				
	464.2	24.00	51.70	81.3	142.0	36.0	60.0
		2*A1+16*A10+4*A12+4*A11+10*A2					[97]
		Forms liquid crystal					
$C_{36}H_{53}NO_5$		17-(cyclopropylmethyl)-α-(1,1-dimethylethyl)-4,5-epoxy-18,19-dihydro-6-methoxy-α-methyl-(1-oxoheptyloxy)-6,14-ethenomorphinan-7-methanol					
	360.0	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]
$C_{36}H_{64}O_4$		2,5-di-*n*-pentadecyloxy-1,4-benzoquinone					
	385.9	21.7	56.23				
	393.5	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]
$C_{36}H_{74}O_{16}$		54-crown-18					
	317.2	81.6		257.2	243.7	81.6	77.3

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

	T (K)	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (expt)	$\Delta_0^{T_{fus}} S_{tpce}$ (calcd)	$\Delta_0^{T_{fus}} H_{tpce}$ (expt)	$\Delta_0^{T_{fus}} H_{tpce}$ (calcd)
		$A14+51*A15+18*A112$					[386]
$C_{36}H_{74}O_{18}$		1,ω-dimethoxyheptadeca(oxyethylene)					
	301.2	136.6		453.5	436.2	136.6	131.4
		$2*A1+34*A2*B2+18*A32$					[386]
$C_{36}H_{75}AsO_2$*		di-*n*-nonadecylarsinic acid					
	394	128.9		327.2	327.4	128.9	129.0
		$2*A1+34*A2*B2+A142$					[381]
$C_{38}H_{68}O_4$		2,5-di-*n*-hexadecyloxy-1,4-benzoquinone					
	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	133.0
		$2*A1+30*A2*B2+A14+3*A15+2*A18+2*A19+2*A32+2*A114$					[342]
$C_{38}H_{78}O_{19}$		1,ω-dimethoxyoctadeca(oxyethylene)					
	305.2	156.7		513.5	459.5	156.7	140.2
		$2*A1+36*A2*B2+19*A32$					[386]
$C_{40}H_{40}N_2O_4$*		3,3′,4,4′-biphenyltetracarboxy-N,N′-bis-(4-*n*-hexylphenyl)diimide					
	432.4	19.9	46.02				
	513.8	26.2	50.99				
	563.3	9.50	16.86	113.9		55.60	
		No prediction made. Forms liquid crystal					[87]
$C_{40}H_{50}$*		1,8-*bis*[4(4′-*n*-butylbiphenyl)]octane					
	398.2	13.0	32.65				
	414.2	27.0	65.19	97.2	184.6	40.0	76.5
		$2*A1+16*A10+4*A12+4*A11+14*A2$					[97]
		Forms liquid crystal					
$C_{40}H_{72}O_4$		2,5-di-*n*-heptadecyloxy-1,4-benzoquinone					
	383.6	13.0	33.89				
	395.3	120.9	305.8	339.7	353.1	133.9	139.6
		$2*A1+32*A2*B2+A14+3*A15+2*A18+2*A19+2*A32+2*A114$					[342]
$C_{42}H_{44}N_2O_4$*		3,3′,4,4′-biphenyltetracarboxy-N,N′-bis-(4-*n*-heptylphenyl)diimide					
	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]
$C_{44}H_{48}N_2O_4$*		3,3′,4,4′-biphenyltetracarboxy-N,N′-bis-(4-*n*-octylphenyl)diimide					
	428.5	36.10	84.25				
	499.2	21.30	42.67				
	553.5	8.50	15.36	142.3		65.9	
		Forms liquid crystal					[87]
$C_{44}H_{80}O_4$		2,5-di-*n*-nonadecyloxy-1,4-benzoquinone					
	385.5	16.2	42.0				
	396.2	134.0	338.2	380.2	390.5	150.2	154.7
		$2*A1+36*A2*B2+A14+3*A15+2*A18+2*A19+2*A32+2*A114$					[342]
$C_{44}H_{90}$		*n*-tetratetracontane					
	360.9	145.5		403.1	425.8	145.5	153.7
		$2*A1+42*A2*B2$					[210]
$C_{50}H_{102}$		*n*-pentacontane					
	366.9	185.0		504.2	481.6	185.0	176.7
		$2*A1+48*A2*B2$					[210]
$C_{52}H_{106}O_{26}$		1,ω-dimethoxypentacosa(oxyethylene)					
	316.2	209.7		663.3	622.7	209.7	196.9
		$2*A1+50*A2*B2+26*A32$					[386]
$C_{54}H_{108}O_{27}$		81-crown-27					
	314.2	155.6		495.4	354.4	155.6	111.3
		$A14+78*A15+27*A112$					[386]
$C_{56}H_{114}O_{28}$		1,ω-dimethoxyheptacosa(oxyethylene)					
	315.2	224.6		712.6	669.3	224.6	210.9
		$2*A1+54*A2*B2+28*A32$					[386]
$C_{92}H_{186}O_{46}$		1,ω-dimethoxypentatetracosa(oxyethylene)					
	324.2	374.8		1156.3	1089.0	374.8	353.0
		$2*A1+90*A2*B2+46*A32$					[386]
$C_{100}H_{202}$		*n*-hectane					
	365.5	54.8	149.9				
	388.5	331.8	854.1	1004.0	946.7	386.8	368.8
		$2*A1+98*A2*B2$					[343]
$C_{192}H_{386}$		*n*-dononacontahectane					

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

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

[a]Units for $\Delta_0^{T_{fus}} S_{tpce}$ and $\Delta_0^{T_{fus}} H_{tpce}$ 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 table, some of these compounds exhibit liquid crystal behavior, others display amphiphillic 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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