Estimating Solid–Liquid Phase Change Enthalpies and Entropies

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

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1. Introduction

1.1. Fusion Enthalpies

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

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

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

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, $T_{\rm fus}$, is a group property and that this property can be estimated by standard group additivity techniques. The total phase change entropy has been defined as the sum of the entropy associated with all the phase changes occurring in the condensed phase prior to and including melting. The assumption that the total phase change entropy is a more reliable group property than fusion entropy is readily apparent from an examination of these two properties as a function of the number of methylene groups for the *n*-alkanes. This is illustrated in Figs. 1 and 2. Many alkanes have additional phase transitions with significant entropy components that influence the magnitude of the fusion entropy. This leads to the nonlinear behavior illustrated in Fig. 1. When these components are added together, the total phase change entropy shows a much better linear correlation. Some odd–even alternation as a function of the number of carbon atoms is evident similar to what is observed in the melting points of these compounds

2. Estimation of Total Phase Change Entropy and Enthalpy

2.1. Derivation of Group Values

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

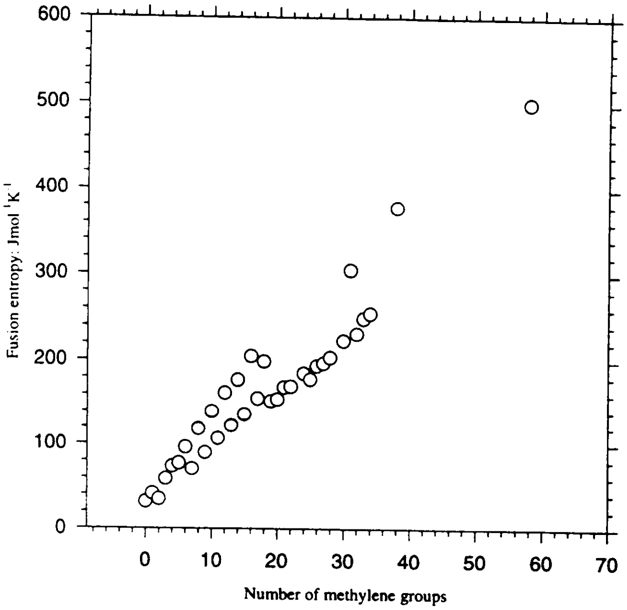


FIG. 1. Fusion entropy of the n-alkanes as a function of the number of methylene groups.

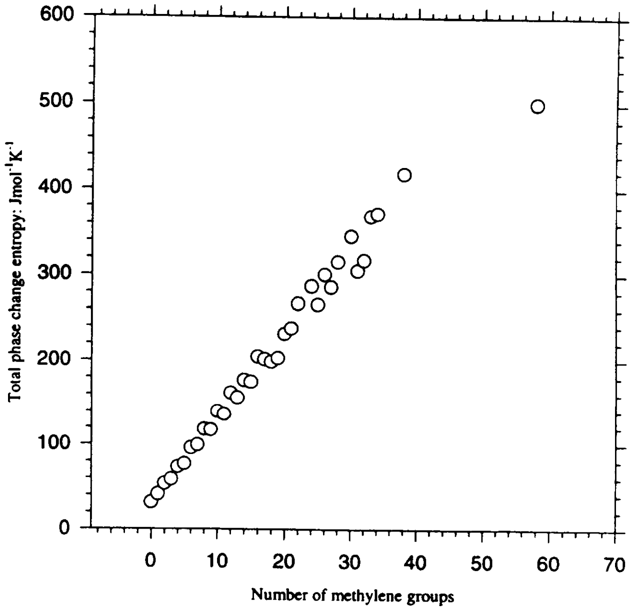


FIG. 2. Total phase change entropies of the n-alkanes as a function of the number of methylene groups.

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

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

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

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

A listing of the group parameters that can be used to estimate these phase change properties is presented in Tables 1 and 2. The group values in these tables have been updated from previous versions by the inclusion of new experimental data in the parameterizations.[8,9] Before describing the application of these parameters in the estimation of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$, the conventions used to describe these group values need to be defined. Primary, secondary, tertiary, and quaternary centers, as found on atoms of carbon, silicon, and their congeners, are defined solely on the basis of the number of hydrogens attached to the central atom, 3, 2, 1, 0, respectively. It should be noted that the experimental melting point along with an estimated value of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ is necessary to estimate the fusion enthalpy of a compound. In addition, compounds whose liquid phase is not isotropic at the melting point are not modeled properly by these estimations. Those compounds forming liquid crystal or cholesteric phases as well amphiphilic compounds are currently overestimated by these parameters. A large discrepancy between the estimated total phase change enthalpy and experimental fusion enthalpy is a good indication of undetected solid–solid phase transitions or anisotropic liquid behavior.

The parameters used for estimating $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ of hydrocarbons and the hydrocarbon portions of more complex molecules are listed in Table 1. The group value, G_i, associated with a molecular fragment is identified in the third column of the table. The group coefficients, C_i, are listed in column 4 of the table. These group coefficients are used to modify G_i whenever a functional group is attached to the carbon in question. Functional groups are defined in Table 2. Group values reported in parenthesis are based on only a limited database (arbitrarily chosen as less 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_{CH_2}, is applied differently from the rest and its application is discussed below. Introduction of this coefficient is new and differentiates this protocol 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 $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ 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:

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

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

$$i\neq{\rm CH_2} \quad \text{otherwise } C_{\rm CH_2}=1. \qquad (2)$$

The group coefficient for a methylene group $C_{\rm CH_2}$ is used whenever the total number of consecutive methylene groups in a molecule $n_{\rm CH_2}$ 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 $C_{\rm CH_2}$ is provided in the discussion that pertains to polymers below. Entries for each estimation in Table 3 include the melting point $T_{\rm fus}$ 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 $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ and $T_{\rm fus}$ is followed by the experimental total phase change enthalpy (or fusion enthalpy). Finally, details in estimating $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ 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 $\rm J{\cdot}mol^{-1}{\cdot}K^{-1}$ and together with the experimental melting point, an enthalpy of fusion of 12.6 $\rm kJ{\cdot}mol^{-1}$ is estimated. This can be compared to the experimental value of 11.0 $\rm kJ{\cdot}mol^{-1}$. 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 $C_{\rm CH_2}$ 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 ($C_{\rm CH_2}=1.0$) 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 $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ for acenaphthylene will be illustrated below.

3.2. Nonaromatic Cyclic and Polycyclic Hydrocarbons

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

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

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

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

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

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, $\Delta_0^{T_{\rm fus}}S_{\rm tpce}(corr)$. 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 $\Delta_0^{T_{\rm fus}}S_{\rm tpce}(corr)$. These additional acyclic and/or aromatic terms $[\Delta_0^{T_{\rm fus}}S_{\rm tpce}(aah)]$ are added according to the protocol discussed above in the use of Eq. (2). The following examples of Table 3 illustrate the use of Eq. (3) and (4) according to Eq. (5) to estimate the total phase change entropy of cyclic molecules $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(total)$:

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

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

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

3.2.2. Bullvalene

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

3.2.3. Acenaphthylene

Estimation of $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ and $\Delta_0^{T_{\text{fus}}}H_{\text{tpce}}$ for acenaphthylene completes this section on cyclic hydrocarbons. Molecules that contain rings fused to aromatic rings but are not completely aromatic, according to the definition provided above, are estimated by first calculating $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}$ *(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 $\{\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(ring):[33.4]+2[3.7]\}$ is first adjusted for each nonsecondary sp^3 carbon atom in the ring $\{\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(corr):+2[-1.6]+3[-12.3]\}$, and then the remainder of the aromatic portion of the molecule is added $\{\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(aah):[-7.5]+6[7.4]\}$. 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 $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(total)$ for acyclic and aromatic derivatives and for cyclic and polycyclic hydrocarbon derivatives, respectively,

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

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

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

4.1.3. Trifluoroacetonitrile

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

4.1.4. Isoquinoline

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

4.2. Cyclic and Polycyclic Hydrocarbon Derivatives

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

↳ TABLE 4B is in caps see pg 13

4.2.1. 2-Chlorodibenzodioxin

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

4.2.2. 6,8,9-Trimethyladenine

6,8,9-Trimethyladenine is estimated in a similar fashion. The ring equation [Eq. (3)] is used first to generate the contribution of the five membered heterocyclic ring. In this instance the ring has been modified by the addition of a cyclic sp^2 hybridized nitrogen atom and a nitrogen which comprises part of a cyclic tertiary amine. Both ring substitutions require appropriate corrections. The hybridization and substitution of the remaining three cyclic carbon atoms of the five membered ring have likewise been changed from the pattern found in cyclopentane and appropriate changes must also be included in $\Delta_0^{T_{\text{fus}}}S_{\text{tpce}}(corr)$. 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 $\Delta_0^{T_{\mathrm{fus}}}S_{\mathrm{tpce}}$ of small molecules, the parameters of Tables 1 and 2 can be used to predict $\Delta_0^{T_{\mathrm{fus}}}S_{\mathrm{tpce}}$ and $\Delta_0^{T_{\mathrm{fus}}}H_{\mathrm{tpce}}$ (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 $\Delta_0^{T_{\mathrm{fus}}}S_{\mathrm{tpce}}$ 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 $(\mathrm{CH_2O})_n$, is treated as an infinite chain with $n_0 = n_{\mathrm{CH_2}}$. For a molecule such as $\mathrm{CH_3O(CH_2CH_2O)}_n\mathrm{CH_3}$, 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 $\Delta_0^{T_{\mathrm{fus}}}S_{\mathrm{tpce}}$ 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 $C_{\mathrm{CH_2}}$ 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]

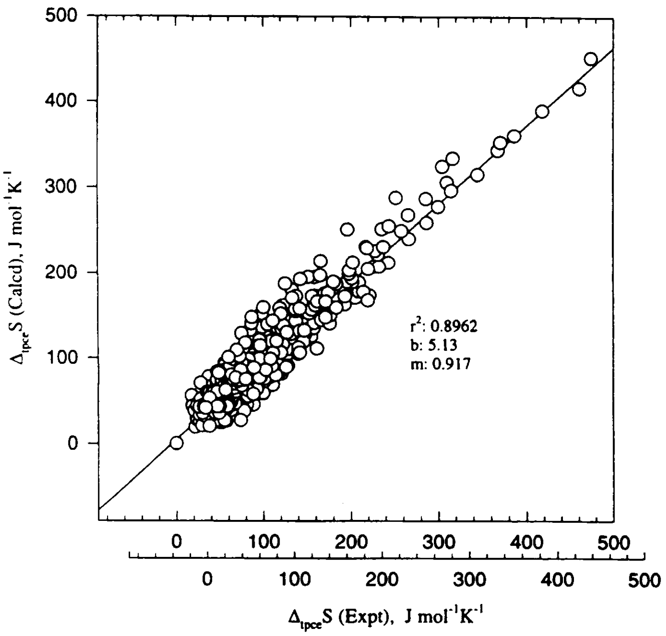


FIG. 3. A comparison of calculated and experimental $\Delta_0^{T_{fus}}S_{tpce}$ of 1858 database compounds.

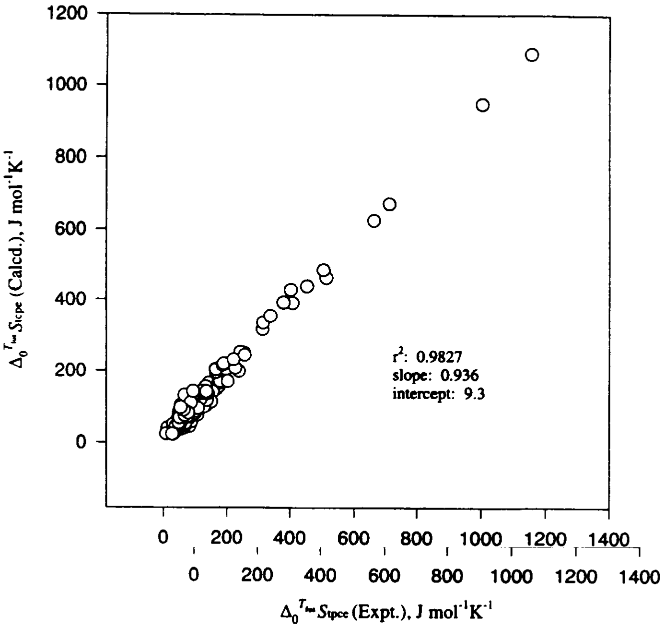


FIG. 5. A comparison of calculated and experimental $\Delta_0^{T_{fus}}S_{tpce}$ of 260 test compounds.

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. tal enthalpies associated with all solid–solid and solid–liquid

phase changes (ΔH_{pce}, column 2), the corresponding phase

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 experimental and calculated total phase change entropies for

the database are compared in Fig. 3. The correlation was

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

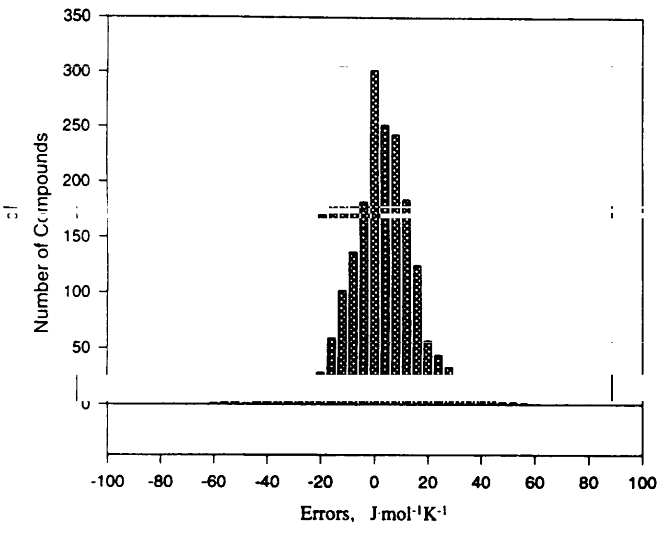


FIG. 4. A histogram illustrating the distribution of errors in estimating $\Delta_0^{T_{fus}}S_{tpce}$ of the database compounds.

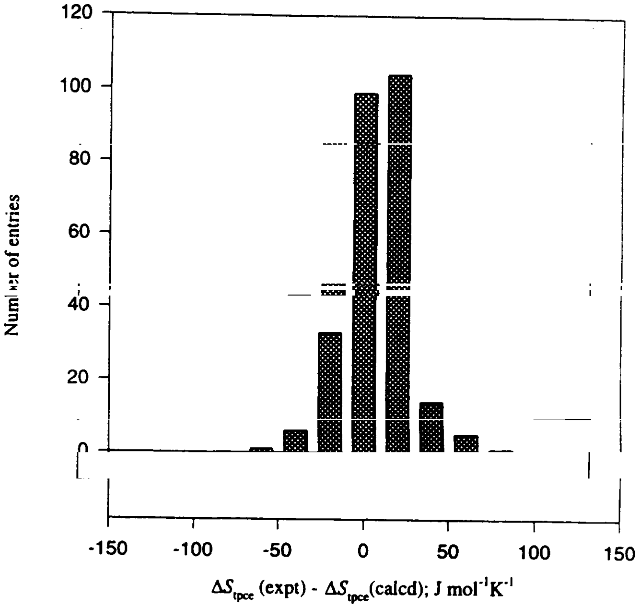


FIG. 6. A histogram illustrating the distribution of errors in estimating $\Delta_0^{T_{fus}}S_{tpce}$ of 260 test compounds.

calculated $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ and $\Delta_0^{T_{\rm fus}}H_{\rm tpce}$ values for these 1858 compounds are 9.9 $\rm J\cdot mol^{-1}\cdot K^{-1}$ and 3.52 $\rm kJ\cdot mol^{-1}$, and 0.154 and 0.17, respectively. The standard deviations between experimental and calculated values for $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ and $\Delta_0^{T_{\rm fus}}H_{\rm tpce}$ are $\pm 13.0\,\rm J\cdot mol^{-1}\cdot K^{-1}$ and $\pm 4.88\,\rm kJ\cdot mol^{-1}$, 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 $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ and $\Delta_0^{T_{\rm fus}}H_{\rm tpce}$ were $\pm 18.4\,\rm J\cdot mol^{-1}\cdot K^{-1}$ and $\pm 7.2\,\rm kJ\cdot mol^{-1}$, respectively. The absolute average and relative errors between experimental and calculated $\Delta_0^{T_{\rm fus}}S_{\rm tpce}$ and $\Delta_0^{T_{\rm fus}}H_{\rm tpce}$ values for these 260 compounds were 13.9 $\rm J\cdot mol^{-1}\cdot K^{-1}$ and 5.28 $\rm kJ\cdot mol^{-1}$, 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 ($\rm J\cdot mol^{-1}\cdot K^{-1}$)		Group coefficients[a] C_i	
primary sp^3	$\rm CH_3$–	17.6	(*A*1)		
secondary sp^3	$\rm >CH_2$	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	$\rm =CH_2$	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	$\rm =C_aH$–	7.4	(*A*10)		
quaternary aromatic sp^2 carbon adjacent to an sp^3 atom	$\rm =C_a(R)$–	−9.6	(*A*11)		
peripheral quaternary aromatic sp^2 carbon adjacent to an sp^2 atom	$\rm =C_a(R)$–	−7.5	(*A*12)		
internal quaternary aromatic sp^2 carbon adjacent to an sp^2 atom	$\rm =C_a(R)$–	−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 $\rm C_{CH_2}$ 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) ($\rm J\cdot mol^{-1}\cdot K^{-1}$)		Group coefficient C_i	
cyclic tertiary sp^3	$>\rm C_cH(\mathit{R})$	−14.7	(*A*16)		
cyclic quaternary sp^3	$>\rm C_c(\mathit{R})_2$	−34.6	(*A*17)		
cyclic tertiary sp^2	$\rm =C_cH$–	−1.6	(*A*18)	1.92	(*B*18)
cyclic quaternary sp^2	$\rm =C_c(\mathit{R})$–	−12.3	(*A*19)		
cyclic quaternary sp	$\rm =C_c=$; $R\rm -C_c\equiv$	−4.7	(*A*20)		
Ring equations for nonaromatic cyclic compounds					
$\Delta S_{\rm ring}=[33.4(A14)]+[3.7(A15)][n-3]$;	n = number of ring atoms				
Ring equation for nonaromatic polycyclic compounds					
$\Delta S_{\rm ring}=[33.4(A14)]N+[3.7(A15)][R-3N]$;	R = total number of ring atoms; N = number of rings				

please move as suggested so numbers are in sequence

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

Functional groups[a]	Group value (G_k)[a] J/(mol K)			Group coefficient (C_k)[b] k				
				2	3	4	5	6
bromine	R–Br	17.5	(*A21*)					
chlorine	R–Cl	10.8	(*A22*)	1.5 (*B22*)	1.5 (*C22*)	1.5 (*D22*)	1.5 (*E22*)	1.5 (*F22*)
fluorine on an sp^2 carbon	═CRF	19.5	(*A23*)					
fluorine on an aromatic carbon	═CF–	16.6	(*A24*)					
3-fluorines on an sp^3 carbon	CF_3–R	13.3	(*A25*)					
2-flurorines on an sp^3 carbon	R—CF_2–R	16.4	(*A26*)					
1-fluorine on an sp^3 carbon	R—CF–$(R)_2$	12.7	(*A27*)					
fluorine on a ring carbon	–CHF–	[17.5]	(*A28*)					
	–CF_2–	[17.5]	(*A28*)					
iodine	R–I	19.4	(*A29*)					
hydroxyl group	R–OH	1.7	(*A30*)	10.4 (*B30*)	9.7 (*C30*)	13.1 (*D30*)	12.1 (*E30*)	13.1 (*F30*)
phenol	═C–(OH)–	20.3	(*A31*)					
ether	R—O–R	4.71	(*A32*)					
peroxide, 1	R–O–O–R	[10.6]	(*A33*)					
aldehyde	R–CH(═O)	21.5	(*A34*)					
ketone	R–C(═O)–(R)	4.6	(*A35*)					
carboxylic acid	R–C(═O)OH	13.4	(*A36*)	1.21 (*B36*)	2.25 (*C36*)	2.25 (*D36*)	2.25 (*E36*)	2.25 (*F36*)
formate ester	R–OCH(═O)	[4.2]	(*A37*)					
ester	R–C(═O)O–R	7.7	(*A38*)					
anhydride	R–C(═O)OC(═O)–R	[10.0]	(*A39*)					
acyl chloride	R–C(═O)Cl	[25.8]	(*A40*)					
aromatic heterocyclic amine	═N–	[10.9]	(*A41*)					
acyclic sp^2 nitrogen	═N–	[−1.8]	(*A42*)					
tertiary amine	R–N(R_2)	−22.2	(*A43*)					
secondary amine	R–NH–R	−5.3	(*A44*)					
primary amine	R–NH_2	21.4	(*A45*)					
azide	R–N_3	[−32.5]	(*A46*)					
tertiary amine *N*-nitro	R_2–N–(NO_2)	5.39	(*A47*)					
aliphatic secondary amine *N*-nitro	R–NH–(NO_2)	[−4.59]	(*A48*)					
aromatic tertiary amine-*N*-nitro	R–NH–(NO_2)	[−41.7]	(*A49*)					
nitro group	R–NO_2	17.7	(*A50*)					
N-nitro	>N–(NO_2)	39.8	(*A51*)					
N-nitroso	>N–N═O	[28.6]	(*A52*)					
oxime	═N–OH	[13.6]	(*A53*)					
azoxy nitrogen	N═N(→O)–	[6.8]	(*A54*)					
nitrate ester	R–ONO_2	[24.4]	(*A55*)					
nitrile	R–C≡N	17.7	(*A56*)					
isocyanide	R–NC	[17.5]	(*A57*)					
isocyanate	R–N═C═O	[23.1]	(*A58*)					
tertiary amides	R–C(═O)NR_2	−11.2	(*A59*)					
secondary amides	R–C(═O)NH–R	1.5	(*A60*)					
primary amide	R–$CONH_2$	27.9	(*A61*)					
N,N-dialkylformamide, 1	HC(═O)NR_2	[6.9]	(*A62*)					
tetra substituted urea	R_2NC(═O)NR_2	[−19.3]	(*A63*)					
1,1,3-trisubst urea	R_2NC(═O)NH–R	[0.2]	(*A64*)	−12.8 (*B64*)	−24 (*C64*)	6 (*D64*)		
1,1-disubstituted urea	R_2NC(═O)NH_2	[19.5]	(*A65*)					
1,3-disubstituted urea	RNHC(═O)NH–R	[1.5]	(*A66*)					
mono substituted urea	R–NHC(═O)NH_2	[22.5]	(*A67*)					
N,N-disubstituted carbamate	R–OC(═O)NR_2	−23.12	(*A68*)					
N-substituted carbamate	R–OC(═O)NH–R	10.6	(*A69*)					
carbamate	R–OC(═O)NH_2	[27.9]	(*A70*)					
imide	R–C(═O)NHC(═O)–R	[7.7]	(*A71*)					
phosphine	R_3–P	[−20.7]	(*A72*)					
phosphine oxide	R_3–P═O	[−32.7]	(*A73*)					
phosphate ester	P(═O)(O–R)$_4$	[−10.0]	(*A74*)					
phosphonate ester	R–P(═O)(O–R)$_2$	[−14.0]	(*A75*)					
phosphonic acid	R–P═O(OH)$_2$	[7.7]	(*A76*)					
phosphonyl halide	R–P(═O)X_2	[4.8]	(*A77*)					

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

Functional groups[a]	Group value (G_k)[a] J/(mol K)			Group coefficient (C_k)[b] k				
				2	3	4	5	6
phosphoramidate ester	$(R-O)_2P(=O)NH-R$	[−0.7]	(A78)					
phosphorothioate ester	$(R-O)_3P(=S)$	1.1	(A79)					
phosphorodithioate ester	$R-S-P(=S)(O-R)_2$	−9.6	(A80)					
phosphonothioate ester	$R-P(=S)(O-R)_2$	[5.2]	(A81)					
phosphoroamidothioate ester	$R-NHP(=S)(O-R)_2$	[16.0]	(A82)					
phosphoroamidodithioate ester	$NH_2P(=S)(S-R)(O-R)$	[6.9]	(A83)					
sulfides	$R-S-R$	2.1	(A84)					
disulfides	$R-SS-R$	9.6	(A85)					
thiols	$R-SH$	23.0	(A86)					
sulfoxide	$R-S(\rightarrow O)-R$	[14.1]	(A87)					
sulfones	$R-S(\rightarrow O)_2-R$	0.3	A88)					
sulfonate ester	$R-S(\rightarrow O)_2O-R$	[7.9]	(A89)					
1,2-disubstituted thiourea	$R-NHC(=S)NH-R$	[14.4]	(A90)					
monosubst thiourea	$R-NHC(=S)+NH_2$	[23.1]	(A91)					
thioamide	$R-C(=S)NH_2$	[30.0]	(A92)					
N,N disubstituted thiocarbamate	$R-S(C=O)N-R_2$	[5.6]	(A93)					
N,N-disubstituted sulfonamide	$R-S(\rightarrow O)_2N-R_2$,	[−11.3]	(A94)					
N-substituted sulfonamide	$R-S(\rightarrow O)_2NH-R$	6.3	(A95)					
sulfonic acid	$R-S(\rightarrow O)_2OH$	[1.8]	(A145)					
sulfonamide	$R-S(\rightarrow O)_2NH_2$	[28.4]	(A96)					
trisubstituted aluminum	R_3-Al	[−24.7]	(A97)					
trisubstituted arsenic	R_3-As	[−6.5]	(A98)					
trisubstituted boron	R_3-B	[−17.2]	(A99)					
trisubstituted bismuth	R_3-Bi	[−14.5]	(A100)					
trisubstituted galium	R_3-Ga	[−11.9]	(A101)					
tetrasubstituted germanium	R_4-Ge	[−35.2]	(A102)					
disubstituted germanium	R_2GeH_2	[−14.7]	(A103)					
disubstituted mercury	R_2-Hg	[8.4]	(A104)					
trisubstituted indium	R_3-In	[−19.3]	(A105)					
tetrasubstituted lead	R_4-Pb	[−30.2]	(A106)					
trisubstituted antimony	R_3-Sb	[−12.7]	(A107)					
disubstituted selenium	R_2-Se	[6.0]	(A108)					
quaternary silicon	R_4-Si	−27.1	(A109)					
quaternary tin	R_4-Sn	−24.2	(A110)					
disubstituted zinc	R_2-Zn	[11.1]	(A111)					
disubstituted telluride	R_2-Te	[−2.2]	(A140)					
trisubstituted germanium	R_3-GeH	[−27.8]	(A141)					
disubstituted arsinic acid	R_2-AsO_2H	[−24]	(A142)					
trisubstituted thallium	R_3-Th	[1]	(A143)					
disubstituted cadmium	R_2-Cd	[−2]	(A144)					

[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.

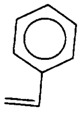
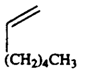
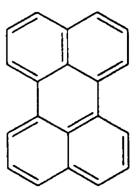
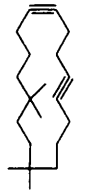
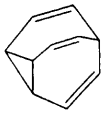
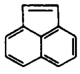
TABLE 2. (b) Contributions of functional groups as part of a ring

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

[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]

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

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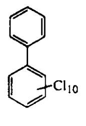
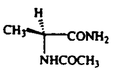
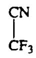
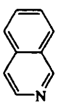
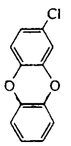
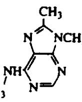
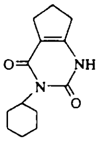
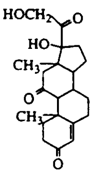
[a] Units for $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ are $J \cdot mol^{-1} \cdot K^{-1}$ and $kJ \cdot mol^{-1}$, respectively; experimental values are included in parentheses following the calculated value (in cases where additional solid–solid transitions are involved, the first 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

Compound	Structure	T_{fus}	$\Delta_0^{T_{fus}}S_{tpce}$	$\Delta_0^{T_{fus}}H_{tpce}$	$\Delta_0^{T_{fus}}S_{tpce}$
A. Substituted Aromatic and Aliphatic Molecules[a]					
$C_{12}Cl_{10}$ decachlorobiphenyl[b]		577.7 K	72.1 (68.1)	41.6 (39.3)	{~~10~~2[-7.5]+ {10[1.5][10.8]}
$C_5H_{10}N_2O_2$ N-acetyl-L-alanine amide[c]		431 K	54.9 (50.4)	23.7 (21.7)	{2[17.6]+ [27.9]+0.6[-16.4]+[1.5]}
C_2F_3N 2,2,2-trifluoroacetonitrile[c]	 CF_3CN	128.7 K	34.6 (38.6)	4.5 (5.0)	{[-34.8][0.66] 3[13.3]+[17.7]}
C_9H_7N isoquinoline[c]		299.6 K	47.9 (52.1)	14.3 (13.5)	{[10.9]+7[7.4]+ 2[-7.5]}
B. Substituted Cyclic Molecules[a]					
$C_{12}H_7ClO_2$ 2-chlorodibenzodioxin[d]		362.2 K	58.5 (63.8)	21.2 (23.1)	{[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]		438 K	54.3 (52.7)	23.8 (23.1)	{[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]		584.3 K	64.0(72.4)	37.4 (42.3)	{3[33.4] + 6[3.7]+2[-12.3]+ [-14.7]+[-21.7] [2.7]}
$C_{21}H_{28}O_5$ cortisone[f]		495 K	75.2 (74.5)	37.2 (36.9)	{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]}

✓ 12
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✓

[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] ~~Acree, 1991~~. 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)	$\Delta_0^{T_\text{fus}} S_\text{tpce}$ (expt)	$\Delta_0^{T_\text{fus}} S_\text{tpce}$ (calcd)	$\Delta_0^{T_\text{fus}} H_\text{tpce}$ (expt)	$\Delta_0^{T_\text{fus}} H_\text{tpce}$ (calcd)
	205	0.21	1.02				
	223.6	7.45	33.31				
	240.1	1.88	7.84	42.17	43.3	9.54	10.4
	224.2	7.47	33.3				
	240.2	1.88	7.8	41.1		9.4	
	224.8	7.49	33.3				
	243.1	2.35	9.67	43.0		9.8	
		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	
		$A1+A61$					[271,216]
$C_2H_5NO_2$		nitroethane					
	183.7	9.85	0	53.64	42.4	9.85	7.8
		$A1+A2+A50$					[216]
$C_2H_5NO_2$		methyl carbamate					
	328.6	16.7	0	50.82	45.5	16.7	14.9
		$A1+A70$					[216]
$C_2H_5NO_3$		ethyl nitrate					
	178.6	8.53	0	47.74	49.1	8.53	8.8
		$A1+A2+A55$					[126]
C_2H_5NS		ethanethioamide					
	385.7	18.36	0	47.59	47.6	18.36	18.4
		$A1+A92$					[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	
		$2*A1$					[216]
$C_2H_6ClO_3P$		2-chloroethylphosphonic acid					
	347.9	14.79	0	42.51	42.6	14.79	14.8
		$2*A2+A22*B22+A76$					[221]
$C_2H_6Cl_2Si$		dimethyldichlorosilane					
	199.0	8.83	0	44.36	40.5	8.83	8.1
		$2*A1+2*A22*C22+A109$					[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	
		$A1+A67$					[138.216]
$C_2H_6N_2O_2$		N-nitro-N-methylaminomethane					
	327	37.66	0	115.16	80.3	37.66	26.3
		$2*A1+A51+A47$					[225]
$C_2H_6N_4O_4$		N.N′-dinitroethanediamine					
	450	29.5	0	65.55	84.6	29.5	38.07
		$2*A2+2*A48+2*A51$					[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	
		$A1+A2+A30$					[216]
C_2H_6O		dimethyl ether					
	131.7	4.94	0	37.5	39.9	4.94	5.3
		$2*A1+A32$					[216]
C_2H_6OS		dimethyl sulfoxide					
	291.7	14.37	0	49.26	49.3	14.37	14.4
		$2*A1+A87$					[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	
		$2*A2+2*A30*B30$					[216]
$C_2H_6O_2S$		dimethylsulfone					
	382	18.28	0	47.91	35.4	18.30	13.5
		$2*A1+A88$					[216]
C_2H_6S		ethyl mercaptan					
	195.3	4.97	0	25.48	47.7	4.97	9.3
		$A1+A2+A86$					[216]
C_2H_6S		dimethyl sulfide					
	174.9	7.98	0	45.66	37.3	7.98	6.5
		$2*A1+A84$					[216]
$C_2H_6S_2$		dimethyldisulfide					
	188.4	9.19	0	48.78	44.7	9.19	8.4
		$2*A1+A85$					[216]
C_2H_6Se		dimethylselenium					
	185.1	8.5	0	45.91	41.1	8.5	7.6
		$2*A1+A108$					[170]
$C_2H_6Se_2$		dimethyldiselenium					
	190.8	8.55	0	44.78	47.1	8.55	9.0
		$2*A1+2*A108$					[170]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (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
		A14+3*A15+3*A120+3*A52					[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
		A14+A15*3+3*A120+2*A51+A52					[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
		A14+A15*3+3*A120+3*A51					[216]
C_3H_6O		acetone					
	176.6	5.72	0	32.34	39.7	5.72	7.0
		2*A1+A35					[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	
		A1+A14+A112+A16					[216]
C_3H_6O		propanal					
	171.3	8.59	0	50.14	46.3	8.59	7.9
		A1+A2+A34					[216]
$C_3H_6O_2$		propionic acid					
	252.7	10.66	0	42.2	38.1	10.66	9.6
		A1+A2+A36					[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
		A14+2*A15+2*A112					[216]
$C_3H_6O_2$		methyl acetate					
	174.9	7.49	0	42.82	42.8	7.49	7.5
		2*A1+A38					[1]
$C_3H_6O_2S$		β-thiolactic acid					
	291.9	16.97	0	58.15	53.4	16.97	15.6
		2*A2+A36+A86					[216]
$C_3H_7O_3$		DL lactic acid					
	289.9	11.34	0	39.12	42.2	11.34	12.2
		A1+A3*B3+B30*A30+A36*B36					[216]
$C_3H_6O_3$		1,3,5-trioxane					
	333.4	15.11	0	45.3	48.2	15.11	16.1
		A14+3*A15+3*A112					[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
		A14+A15+A131					[216]
C_3H_7Br		2-bromopropane					
	184.1	6.53	0	35.5	43.1	6.53	7.9
		2*A1+A3*B3+A21					[216]
C_3H_7Cl		2-chloropropane					
	156	7.39	0	47.37	36.3	7.39	5.7
		A3*B3+2*A1+A22					[215]
C_3H_7N		cyclopropylamine					
	237.8	13.18	0	55.44	40.0	13.18	9.5
		A14+A45+A16					[215]
C_3H_7NO		N,N-dimethylformamide					
	212.9	8.95	0	42.05	42.1	8.95	9.0
		2*A1+A62					[216]
C_3H_7NO		N-methylacetamide					
	303.8	9.73	0	32.01	36.6	9.73	11.1
		2*A1+A60					[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	
		A1+A2+A70					[215, 216]
$C_3H_7NO_3$		isopropyl nitrate					
	190.9	10.1	0	52.9	49.9	10.1	9.5
		2*A1+A3*B3+A55					[173]

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

	$T(K)$	ΔH_{pce} (expt)	ΔS_{pce} (expt)	$\Delta_0^{T_{fus}}S_{tpce}$ (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
		$A2+A3*B3+A1+2*A45$					[50]
$C_3H_{10}N_2$		trimethylhydrazine					
	201.2	9.49	0	47.13	25.2	9.49	5.1
		$3*A1+A44*B44+A43$					[216]
$C_4H_2O_3$		maleic anhydride					
	325.7	12.26	0	37.65	36.9	12.26	12.0
		$A14+2*A15+2*A18*B18+A117$					[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
		$A14+2*A15+A21+A131+2*A18+A18*B18+A19$					[64]
C_4H_3ClS		2-chlorothiophene					
	201.3	8.97	0	44.56	41.3	8.97	8.3
		$A14+2*A15+A22*B22+A131+2*A18+A18*B18+A19$					[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
		$3*A25+2*A26+A1+A38+2*A4*B4$					[216]
$C_4H_4N_2$		pyrazine					
	328.2	12.95	0	39.46	51.5	12.95	16.9
		$4*A10+2*A41$					[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
		$2*A56+2*A2$					[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
		$2*A2+2*A56*C56+A51*C51+A47*C47$					[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
		$A14+2*A15+A112+2*A18*B18+2*A18$					[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
		$3*A15+A14+2*A115$					[216]
$C_4H_4O_4$		ethylene oxalate					
	415	13.4	0	32.29	50.8	13.4	21.1
		$A14+3*A15+2*A115$					[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	
		$A14+2*A15+2*A18*B18+A131+2*A18$					[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
		$A36*B36+A1+A7+A6*B6+B22*A22$					[216]
$C_4H_5ClO_2$		Z-3-chloro-2-butenoic acid					
	366.8	20.71	0	56.48	43.09	20.71	15.81
		$A36*B36+A1+A6*B6+A7+A22*B22$					[216]
$C_4H_5ClO_2$		E-3-chloro-2-butenoic acid					
	333.7	13.81	0	41.38	43.1	13.81	14.4
		$A36*B36+A1+A6*B6+A7+A22*B22$					[216]
C_4H_5N		pyrrole					
	249.7	7.91	0	31.66	33.6	7.91	8.4
		$2*A18+A121+A14+2*A15+2*A18*B18$					[216]
$C_4H_5NO_2$		succinimide					
	400	17.0	0	42.5	42.2	17.0	16.9
		$A14+2*A15+A129$					[216]
C_4H_5NS		2-methylthiazole					
	248.6	12.16	43.44	48.91	43.3	12.16	10.8
		$A14+2*A15+A131+A118+A1+2*A18*B18+A19$					[57, 58]
C_4H_5NS		4-methylthiazole					
	229.1	8.9	0	38.85	43.3	8.9	9.9
		$A14+2*A15+A131+A118+A1+2*A18*B18+A19$					[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)	$\Delta_0^{T_{\mathrm{fus}}} S_{\mathrm{tpce}}$ (expt)	$\Delta_0^{T_{\mathrm{fus}}} S_{\mathrm{tpce}}$ (calcd)	$\Delta_0^{T_{\mathrm{fus}}} H_{\mathrm{tpce}}$ (expt)	$\Delta_0^{T_{\mathrm{fus}}} H_{\mathrm{tpce}}$ (calcd)
	A14+2*A15+A131+A118+A1+2*A18*B18+A19	232.8	7.65	0	32.86	43.3	7.65	10.1 [61]
C_4H_6	1,3-butadiene 2*A5+2*A6	164.2	7.98	0	48.62	45.2	7.98	7.4 [215]
C_4H_6	1,2-butadiene A1+A5+A9+A6	136.9	6.96	0	50.8	37.4	6.96	5.1 [216]
C_4H_6	2-butyne 2*A1+2*A9	240.9	9.25	0	38.38	29.6	9.25	7.1 [215]
C_4H_6	1-butyne A1+A2+A9+A8	147.4	6.03	0	40.9	36.9	6.03	5.4 [216]
$C_4H_6N_6O_8$	1,3,5,5-tetranitro-1,3-diazacyclohexane A14+3*A15+2*A120+2*A51+2*A50+A17	430	29.37	0	68.31	70.8	29.37	30.4 [225,193]
$C_4H_6O_2$	methyl acrylate A1+A5+A6*B6+A38	197.5	9.73	0	49.26	46.5	9.73	9.2 [216]
$C_4H_6O_2$	α-methylacrylic acid A1+A36+A7+A5	287.5	8.06	0	28.04	37.6	8.06	10.8 [216]
$C_4H_6O_2$	*cis*-crotonic acid A1+A6+A36+A6*B6	344.4	12.57	0	36.49	40.1	12.57	13.8 [215]
$C_4H_6O_2$	γ-butyrolactone A14+2*A15+A115	230	9.57	0	41.84	43.9	9.57	10.1 [32]
$C_4H_6O_3$	propylene carbonate 2*A15+A14+A1+A16*B16+A116	218.2	9.62	0	44.07	44.9	9.62	9.8 [89]
$C_4H_6O_4$	dimethyl oxalate 2*A1+2*A38*B38	327.6	21.07	0	64.32	50.5	21.07	16.5 [215]
$C_4H_6O_4$	succinic acid 2*A36*B36+2*A2	457	32.95	0	72.1	46.5	32.95	21.3 [340]
$C_4H_6O_5$	(*dl*) malic acid I A2+2*C36*A36+A3*B3+A30*C30	402	33.52	0	83.39	74.5	33.52	30.0 [216]
$C_4H_6O_5$	(*dl*) malic acid II A2+2*C36*A36+A3*B3+A30*C30	396	30.17	0	76.19	74.5	30.17	29.5 [216]
$C_4H_6O_5$	(*d*) malic acid A3*B3+2*C36*A36+A2+A30*C30	376	23.01	0	61.2	74.5	23.01	28.0 [273]
C_4H_7NO	2-pyrrolidone A14+2*A15+A124	299	13.92	0	46.56	43.5	13.92	13.0 [216]
C_4H_7NO	methacrylamide A1+A7+A5+A61	385.1	15	0	38.95	52.1	15	20.1 [216]
C_4H_8	cyclobutane A14+A15	145.7 182.4	5.71 1.09	39.17 5.96	45.13	37.1	6.79	6.8 [216]
C_4H_8	1-butene A1+A2+A5+A6	87.8	3.85	0	43.84	47.3	3.85	4.2 [216]
C_4H_8	*cis*-2-butene 2*A1+2*A6	134.3	7.31	0	54.43	45.7	7.31	6.1 [216]
C_4H_8	*trans*-2-butene 2*A1+2*A6	167.6	9.76	0	58.22	45.7	9.76	7.7 [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					
C_4H_9Br		1-bromobutane					[216]
	160.4	9.23	57.57	57.57	63.1	9.23	10.1
		3*A2*B2+A21+A1					
C_4H_9Br		*tert*-butyl bromide					[216]
	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					
C_4H_9Br		2-bromobutane					[216]
	160.3	6.88	0	42.92	50.2	6.88	8.0
		2*A1+A2+A3*B3+A21					
C_4H_9Cl		*tert*-butyl chloride					[215]
	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					
C_4H_9N		pyrrolidine					[136]
	207.1	0.54	2.61				
	215.3	8.58	39.84	42.44	43.0	9.12	9.3
		A121+A14+2*A15					
$C_4H_9NO_2$		2-amino-2-methylpropanediol					[216]
	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					
$C_4H_9NO_3$		2-methyl-2-nitro-1-propanol					[274]
	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					
$C_4H_9NO_3$		2-methyl-2-nitro-1,3-propanediol					[216]
	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					
C_4H_{10}		butane					[216]
	107.6	2.07	19.06				
	134.9	4.66	34.56	53.62	49.4	6.73	6.7
		2*A1+2*A2					
C_4H_{10}		isobutane					[216]
	113.7	4.54	0	40.11	36.4	4.54	4.1
		3*A1+A3					
$C_4H_{10}Cl_2Si$		dichlorodiethylsilane					[216]
	174.1	8.96	0	51.45	54.7	8.96	9.5
		2*A22*C22+2*A1+2*A2+A109					
$C_4H_{10}Hg$		diethyl mercury					[216]
	181.5	10.5	0	57.87	57.8	10.5	10.5
		2*A1+A104+2*A2					
$C_4H_{10}N_2O$		N-propylurea					[216]
	381	14.63	0	38.4	54.4	14.63	20.7
		2*A2+A1+A67					
$C_4H_{10}N_2O$		N-isopropylurea					[215]
	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					
$C_4H_{10}N_2O$		1,1,3-trimethylurea					[138]
	344.4	14.3	0	41.52	52.9	14.3	18.2
		3*A1+A64					
$C_4H_{10}N_4O_4$		N-N′dimethyl-N,N′dinitro-1,2-ethanediamine					[215]
	410	60.32	0	147.13	139.7	60.32	57.3
		2*A1+2*A2+2*A51+2*A47					
$C_4H_{10}O$		butyl alcohol					[225]
	183.9	9.28	0	50.46	47.3	9.28	8.7
		3*A2*B2+A1+A30					
$C_4H_{10}O$		2-butanol					[215]
	184.7	5.97	0	32.33	34.4	5.97	6.4
		2*A1+A2+A3*B3+A30					
$C_4H_{10}O$		*tert*-butyl alcohol					[76]
	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]