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Total phase change entropies and enthalpies An update on their estimation and applications to the estimations of amphiphillic fluorocarbon–hydrocarbon molecules

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Abstract

A group additivity method developed to estimate the total phase change entropies and enthalpies of organic solids is updated and the results are compared to the fusion entropies and enthalpies of 547 new measurements. The method is expanded to also include estimations for 58 fluorinated compounds whose liquid phase at the melting point does not behave isotropically. The uncertainties associated with the 547 new measurements, ± 18.6 J mol^{-1} K^{-1} for entropies and ± 7.4 kJ mol^{-1} for enthalpies, are similar in magnitude to those reported previously. Errors associated with estimations for the 58 fluorinated compounds are 16.7 J mol^{-1} K^{-1} and 5.5 kJ mol^{-1}, respectively.

Keywords: Group additivity method; Estimation; Fusion enthalpy and entropy; Amphiphillic hydrocarbons; Total phase change entropy

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 neat aqueous and organic solvents, mixed solvent systems and supercritical fluids. Enthalpy of fusion data adjusted to 298 K, in combination with experimental enthalpies of solution, have been used to calculate the strength of molecular interactions between dissolved crystalline solutes and surrounding solvent molecules [1]. Fusion enthalpy plays an important role in determining molecular packing in crystals and can be useful in correcting thermochemical data to a standard state when combined with other thermodynamic properties [2].

Several thousand new organic and organometallic compounds are synthesized annually. Even with today's modern differential scanning calorimeters, thermal gravimetric analyzers, viscometers, densimeters and other instrumentation, it is impossible to measure the thermodynamic and physical properties of all newly synthesized compounds, let alone the more than six million chemicals already in existence. To address this

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problem, researchers have turned to predictive methods to generate the desired quantities. Given the choice between an estimated or experimental value, selection of the experimental value is clearly preferable. Experimental measurements are not always possible, however, as would be the case in the determination of the enthalpy of fusion for a compound that decomposes upon melting or for a proposed drug molecule that is not yet synthesized. Estimations are also useful in selecting the most probable experimental value in cases where two or more values are in significant disagreement and for identifying single values in need of remeasurement.

Large discrepancies between estimated and experimental 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 non-isotropic molecular motion in the liquid phase. 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 many compounds. The group method reported by Joback and Reid appears to be the most general but is limited by the number of group values available [3]. A few predictive methods have been developed for specific classes of organic compounds, such as saturated triglycerides [4–7] or the *n*-alkanes. Fusion enthalpies have been calculated from fusion entropies and the experimental melting point temperature of the solid (T_{fus}). We recently proposed a general method for estimating total solid–liquid phase change enthalpies and entropies based upon the principles of group additivity [2,8]. The method assumes that unlike fusion enthalpy and entropy, the total phase change entropy associated in going from a rigid solid at 0 K to an isotropic liquid at the melting point (T_{fus}) is a group property and that this property can be estimated by standard group additivity techniques. The phase change entropy is defined as the sum of the entropy associated with all the phase changes occurring in the condensed phase prior to and including melting. In the absence of any solid–solid phase transitions, the total phase change entropy equals the entropy of fusion, $\Delta_{fus}S_m(T_{fus}) = \Delta_{fus}H_m(T_{fus})/T_{fus}$.

At the time of our last publication, we reported group values for 146 different functional groups based upon a regression analysis of experimental enthalpy of fusion data for 1858 organic and organometallic compounds [2]. These group values back-calculated the total phase change entropies ($\Delta_0^{T_{fus}}S_{tpce}$) and enthalpies ($\Delta_0^{T_{fus}}H_{tpce}$) of the 1858 compounds in our database to within absolute average errors of 9.9 J mol^{-1} K^{-1} and 3.52 kJ mol^{-1}, respectively. The standard deviations between experimental and calculated values for $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ were $\pm$13.0 J mol^{-1} K^{-1} and $\pm$4.88 kJ mol^{-1}, and the absolute relative errors were 0.154 J mol^{-1} K^{-1} and 0.17 kJ mol^{-1}, respectively. As an unbiased test of the predictive applicability of the group additivity method, total phase change entropies and enthalpies were predicted for an additional 260 test compounds not included in the original regression analysis. The absolute average and relative errors between experimental and calculated $\Delta_0^{T_{fus}}S_{tpce}$ and $\Delta_0^{T_{fus}}H_{tpce}$ values for these latter 260 compounds were 13.9 J mol^{-1} K^{-1} and 5.28 kJ mol^{-1}, and 0.181 and 0.194, respectively.

Since the publication of our last paper, we have continued to search the chemical and pharmaceutical literature for recently measured enthalpy of fusion data and the older literature for published experimental data that were overlooked during our earlier searches. These efforts have led to the retrieval of enthalpy of fusion data for more than 500 new compounds. The additional enthalpy of fusion data enable the calculation of group parameters for several new functional groups and to modify group values for a few functional groups reported previously. Moreover, the estimation of $\Delta_0^{T_{fus}}S_{tpce}$ for compounds containing fluorine in certain structural environments has been improved and expanded to allow these estimations for diblock perfluorocarbon–perhydrocarbon and related molecules. This is our first attempt at applying a group additivity approach to the estimation of compounds that are not entirely isotropic in the liquid state.

Table 1
Contributions of the hydrocarbon portion of the molecule

Aliphatic and aromatic carbon groups	Group value[a] (G_i, J mol^{-1} K^{-1})	Group coefficient[a] (C_i)
Primary sp^3 C (**CH_3**–R)	17.6 (A1)	
Secondary sp^3 C (R–**CH_2**–R)	7.1 (A2)	1.31[b] (B2)
Tertiary sp^3 C (**CH**(R_3))	−16.4 (A3)	0.60 (B3)
Quaternary sp^3 C (R_4–**C**)	−34.8 (A4)	0.66 (B4)
Secondary sp^2 C (=**CH_2**)	17.3 (A5)	
Tertiary sp^2 C (=**CH**–)	5.3 (A6)	0.75 (B6)
Quaternary sp^2 C (=**C**(R)–)	−10.7 (A7)	
Tertiary sp C (**H**–**C**≡)	14.9 (A8)	
Quaternary sp C (R–**C**≡)	−2.8 (A9)	
Tertiary benzenoid sp^2 C (=**CH**–)	7.4 (A10)	
Quaternary benzenoid sp^2 C adjacent to sp^3 atom[c] (=**C**(R_1)–)	−9.6 (A11)	
Quaternary benzenoid sp^2 C adjacent to sp^2 atom[d] (=**C**(R_2)–)	−7.5 (A12)	
Internal quaternary sp^2 C adjacent to sp^2 atom[e] (=**C**(R_3)–)	−0.7 (A13)	

[a] The alphanumerical terms (A1, A2, B2, etc.) are a device used to identify each group value in the estimations provided in Tables 6–8.
[b] The group coefficient of 1.31 for C_{CH_2} is applied only when the number of consecutive methylene groups excees the sum of the remaining groups; see Section 2.2.1.
[c] This group applies to any quaternary benzenoid carbon adjacent to sp^3 hybridized atom with no lone pair of electrons.
[d] This group applies to any quaternary benzenoid carbon adjacent to any sp^2 hybridized atom and to sp^3 hybridized atoms with non-bonding electrons with the exception of internal quaternary carbon atoms.
[e] Any internal quaternary benzenoid carbon that is not at the periphery of a molecule; for example the six internal quaternary benzenoid carbon atoms of coronene.

2. Estimation of total phase change entropy

2.1. Derivation of new group values

The group values used in estimating the fusion entropies and enthalpies of the new compounds reported in this work are listed in Tables 1–5. Groups that have been changed from our prior work are indicated in column 1 of the tables in bold. The protocol used in these estimations is identical to the one detailed previously with the estimation of fluorinated compounds being the single exception. This protocol is briefly summarized below and includes a discussion of the estimation of compounds containing fluorine. It should also be noted that in the discussions that follows, primary, secondary, tertiary and quaternary carbons are defined by the number of hydrogens attached to carbons 3, 2, 1 and 0, respectively.

2.2. Aliphatic and aromatic compounds

2.2.1. Aliphatic and aromatic hydrocarbons

The estimation of the fusion entropy of hydrocarbons is based solely on the groups present in the

Table 2
Contributions of the functional group portion of the molecule: functional groups dependent on the substitution pattern

Functional groups[a]	Group value[a] (G_k, J mol^{-1} K^{-1})	Group coefficient[a] (C_k)				
		2[b]	3[b]	4[b]	5[b]	6[b]
Chlorine (R–**Cl**)	10.8 (A22)	1.5 (B22)	1.5 (C22)	1.5 (D22)	1.5 (E22)	1.5 (F22)
2-Fluorines on an sp^3 carbon (R–**CF_2**–R)	**13.2 (A26)**	**1.06 (B26)**	**1.06 (C26)**			**1.15**[c] **(F26)**
Hydroxyl group (R–**OH**)	1.7 (A30)	10.4 (B30)	9.7 (C30)	13.1 (D30)	12.1 (E30)	13.1 (F30)
Carboxylic acid (R–**C(=O)OH**)	13.4 (A36)	1.21 (B36)	2.25 (C36)	2.25 (D36)	2.25 (E36)	2.25 (F36)
1,1,3-Trisubstituted urea (R_2**NC(=O)NH**–R)	[0.2] (A64)	−12.8 (B64)	−24 (C64)	6 (D64)		

[a] The alphanumerical terms (A1, A2, B2, etc.) are a device used to identify each group value in the estimations provided in Tables 6–8; the use of the group in bold has been modified from earlier versions; see Section 2.2.2 and Tables 6–8 for examples.
[b] Number of functional groups (k).
[c] To be used in perfluorinated hydrocarbons.

Table 3
Contributions of the functional group portion of the molecule: the remaining functional groups

Functional groups[a]	Group value[b] (G_k, J mol^{-1} K^{-1})
Bromine (R–**Br**)	17.5 (A21)
Fluorine on sp^2 carbon (R_2–CH**F**)	19.5 (A23)
Fluorine on an aromatic carbon (=C**F**–)	16.6 (A24)
3-Fluorines on sp^3 carbon (**CF_3**–R)	13.2 (A25)
1-Fluorine on sp^3 carbon (R–C**F**–(R_2))	12.7 (A27)
Fluorine on a ring carbon (–CH**F**–; –**CF_2**–)	[17.5] (A28); [17.5] (A28)
Iodine (R–**I**)	19.4 (A29)
Phenol (=C–(**OH**)–)	20.3 (A31)
Hydroperoxide (R–**OOH**)	31.8 (A158)
Ether (R–**O**–R)	4.71 (A32)
Peroxide (R–**O**–**O**–R)	[10.6] (A33)
Aldehyde (R–**CH**(=**O**))	21.5 (A34)
Ketone (R–**C**(=**O**)–R)	4.6 (A35)
Formate ester (R–**OCH**(=**O**))	[23.8] (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**)	[−23] (A46)
Tertiary amine-*N*-nitro (R_2–**N**–(NO_2))	[−27.5] (A47)
Aliphatic secondary amine-*N*-nitro (R–**NH**–(NO_2))	[−3.4] (A48)
Aromatic tertiary amine-*N*-nitro (R–**NH**–(NO_2))	[−37.4] (A49)
Nitro group (R–**NO_2**)	17.7 (A50)
***N*-Nitro** (>N–(**NO_2**))	[35.1] (A51)
***N*-Nitroso** (>N–**N**=**O**)	[29.4] (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**)**N**R_2)	−11.2 (A59)
Secondary amides (R–**C**(=**O**)**NH**–R)	1.5 (A60)
Primary amide (R–**C**(=**O**)**NH_2**)	27.9 (A61)
***N*-Alkylformamide** (**HC**(=**O**)**NH**)	[26.4] (A156)
N,*N*-Dialkylformamide (**HC**(=**O**)**NR_2**)	[6.9] (A62)
Tetrasubstituted urea (R_2**NC**(=**O**)**NR_2**)	[−19.3] (A63)
1,1-Disubstituted urea (R_2**NC**(=**O**)**NH_2**)	[19.5] (A65)
1,3-Disubstituted urea (R**NHC**(=**O**)**NH**–R)	[1.5] (A66)
Monosubstituted urea (R–**NHC**(=**O**)**NH_2**)	[16.9] (A67)
N,*N*-Disubstituted carbamate (R–**OC**(=**O**)**NR_2**)	−23.12 (A68)
***N*-Substituted carbamate** (R–**OC**(=**O**)**NH**–R)	7.7 (A69)
Carbamate (R–**OC**(=**O**)**NH_2**)	[27.9] (A70)
Imide (R–**C**(=**O**)**NHC**(=**O**)–R)	[10.4] (A71)

Table 3 (*Continued*)

Functional groups[a]	Group value[b] (G_k, J mol^{-1} K^{-1})
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**($OH)_2$)	[12.1] (A76)
Phosphonyl halide (R–**P**(=**O**)X_2)	[4.8] (A77)
Phosphoramidate ester (($R–O)_2$**P**(=**O**)**NH**–R)	[−0.7] (A78)
Phosphorothioate ester (($R–O)_3$**P**(=**S**))	1.1 (A79)
Phosphorodithioate ester (R–**S**–**P**(=**S**)(**O**–$R)_2$)	−9.6 (A80)
Phosphonothioate ester (R–**P**(=**S**)(**O**–$R)_2$)	[5.2] (A81)
Phosphoroamidothioate ester (R–**NHP**(=**S**)(**O**–$R)_2$)	[16.0] (A82)
Phosphoroamidodithioate ester (**NH_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**(→**O**)–R)	[14.1] (A87)
Sulfones (R–**S**(→**O**)$_2$–R)	0.3 (A88)
Sulfonate ester (R–**S**(→**O**)$_2$**O**–R)	[7.3] (A89)
1,3-Disubstituted thiourea (R–**NHC**(=**S**)**NH**–R)	[3.2] (A90)
Tetrasubstituted thiourea (R_2–**NC**(=**S**)**N**–R_2)	[−7.2] (A148)
Dialkyl-*N*-sulfonylisothiourea (R–**S**–(**C**=**NH**)**NHSO$_2$**R)	[30.0] (A160)
Trialkyl-*N*-sulfonylisothiourea (R–**S**–(**C**=**NR**)**NHSO$_2$**R)	[0.95] (A161)
Monosubstituted thiourea (R–**NHC**(=**S**)**NH_2**)	[28.9] (A91)
Thioamide (R–**C**(=**S**)**NH_2**)	[30.0] (A92)
N,*N*-Disubstituted thiocarbamate (R–**S**(**C**=**O**)**N**–R_2)	[5.6] (A93)
Sulfonic acid (R–**S**(→**O**)$_2$**OH**)	[1.8] (A145)
N,*N*-Disubstituted sulfonamide (R–**S**(→**O**)$_2$**N**–R_2)	[−11.3] (A94)
N-Substituted sulfonamide (R–**S**(→**O**)$_2$**NH**–R)	6.3 (A95)
Sulfonamide (R–**S**(→**O**)$_2$**NH_2**)	[28.4] (A96)
Sulfonyl chloride (R–**S**(→**O**)$_2$Cl)	[25.4] (A157)
Hydrazide (R–**C**(=**O**)**NHNH$_2$**)	[27.3] (A147)
Iminohydrazide (R–**C**(=**O**)**NHN**=CHR)	[18.6] (A159)
Carbonate (R–**OC**(=**O**)**O**–R)	[7.0] (A149)
Trisubstituted aluminum (R_3–**Al**)	[−24.7] (A97)
Trisubstituted arsenic (R_3–**As**)	[−6.5] (A98)
Trisubstituted boron (R_3–**B**)	[−17.2] (A99)
Trisubstituted bismuth (R_3–**Bi**)	[−14.5] (A100)
Trisubstituted gallium (R_3–**Ga**)	[−11.3] (A101)
Tetrasubstituted germanium (R_4–**Ge**)	[−35.2] (A102)
Disubstituted germanium (R_2–**GeH_2**)	[−14.7] (A103)
Disubstituted mercury (R_2–**Hg**)	[8.4] (A104)
Trisubstituted indium (R_3–**In**)	[−19.3] (A105)
Tetrasubstituted lead (R_4–**Pb**)	[−30.2] (A106)
Trisubstituted antimony (R_3–**Sb**)	[−12.7] (A107)
Disubstituted selenium (R_2–**Se**)	[6.0] (A108)
Quaternary silicon (R_4–**Si**)	−27.1 (A109)

Table 3 (*Continued*)

Functional groups[a]	Group value[b] (G_k, J mol^{-1} K^{-1})
Quaternary tin (R_4–**Sn**)	−24.2 (A110)
Disubstituted zinc (R_2–**Zn**)	[11.1] (A111)
Disubstituted tellurium (R_2–**Te**)	[−2.2] (A140)
Trisubstituted germanium (R_3–**GeH**)	[−27.8] (A141)
Disubstituted arsenic acid (R_2–**AsO_2H**)	[−24.0] (A142)
Trisubstituted thallium (R_3–**Tl**)	[1.0] (A143)
Disubstituted cadmium (R_2–**Cd**)	[−2.0] (A144)

[a] The alphanumerical terms (A1, A2, B2, etc.) are a device used to identify each group value in the estimations provided in Tables 6–8; groups in bold in column 1 are new or the value has been changed from earlier versions; see Section 2.2.2 and Tables 6–8 for examples; R: any alkyl or aryl group unless specified otherwise; X: any halogen; units: 18.6 J mol^{-1} K^{-1}; values in brackets are tentative assignments.

[b] All group coefficients; C_k can be assumed to be 1.

molecule according to the following equation:

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

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

$$i \neq CH_2 \text{ otherwise } C_{CH_2} = 1.0 \quad (1)$$

Groups are defined by substitution pattern and hybridization. The terms $n_i G_i$ and $n_{CH_2} G_{CH_2}$ refer to the number of G_i type groups listed in Table 1 and number of methylene groups in the molecule, respectively. For hydrocarbons, all group coefficients (C_i) are equal to 1.0 with one exception. The group coefficient for a methylene group (C_{CH_2}) is equal to 1 unless the number of consecutive methylene groups equals or exceeds the sum of the other groups in the molecule; in the latter case a group coefficient of 1.31 is used. A group coefficient of 1.0 is used for any other methylene groups in the same molecule unless they too exceed this sum. This applies to both hydrocarbons and derivatives. Numerous examples illustrating the application of this protocol can be found in Table 6.

2.2.2. Aliphatic and aromatic hydrocarbon derivatives

Estimations involving derivatives of hydrocarbons consists of three parts: estimation of the contribution of the hydrocarbon component, the estimation of the contribution of the carbon(s) bearing the functional group(s) and the contribution of the functional group(s). The contribution of the hydrocarbon portion of the molecule is estimated as described above. Hydrocarbon group coefficients are all equal to 1.0 or as noted above. The contribution of the carbon bearing the functional group is also evaluated from Table 1. A group coefficient of 1.0 is used unless otherwise indicated by Table 1. The contribution of the functional group is obtained from Tables 2 and 3. The contribution of functional groups listed in Table 2 depends on both the nature of the group (G_k) and the group coefficient (C_k); the group coefficient depends on the total number of functional groups in the molecule. If there is only one functional group in the molecule, $C_{k(1)} = 1.0$.

Fluorine substitution is an exception. The presence of fluorine in a molecule is treated as a single functional group regardless of the number of fluorine atoms present or on their location. Group coefficients for fluorine are also treated differently. Group coefficients for the other functional groups in Table 2 are evaluated on the basis of the total number of functional groups in the molecule. For example, a molecule like 2,2,2-trichloroethanol would be considered to contain a total of four functional groups. The hydroxyl and chlorine functional groups would contribute $C_4 G_{OH}$ and $3C_4 G_{Cl}$ to the total phase change entropy, respectively. 2,2,2-Trifluoroethanol, in contrast, would be considered to contain two functional groups, resulting

Table 4
Contributions of the cyclic hydrocarbon portions of the molecule

Contributions of cyclic carbons	Group value (G_i, J mol^{-1} K^{-1})	Group coefficient (C_i)
Cyclic tertiary sp^3 carbon (–**CH**(R)–)	−14.7 (A16)	
Cyclic quaternary sp^3 carbon (–**C**$(R)_2$–)	−34.6 (A17)	
Cyclic tertiary sp^2 carbon (=**C**H–)	−1.6 (A18)	1.92 (B18)
Cyclic quaternary sp^2 carbon (=**C**(R)–)	−12.3 (A19)	
Cyclic quaternary sp carbon (=**C**=; R–**C**≡)	−4.7 (A20)	

Table 5
Contributions of the cyclic functional groups

Heteroatoms and functional groups comprising a portion of a ring[a,b]	Group value[a] (G_k)
Cyclic ether (*R*–**O**–*R*)	1.2 (A112)
Cyclic peroxide (*R*–**OO**–*R*)	[27.7] (A113)
Cyclic ketone (*R*–**C**(=**O**)–*R*)	−1.4 (A114)
Cyclic ester (*R*–**C**(=**O**)**O**–*R*)	3.1 (A115)
Cyclic carbonate (*R*–**OC**(=**O**)**O**–*R*)	[1.3] (A116)
Cyclic anhydride (*R*–**C**(=**O**)–**O**–**C**(=**O**)–*R*)	2.3 (A117)
Cyclic sp^2 nitrogen (*R*=**N**–*R*)	0.5 (A118)
Cyclic tertiary amine (R_2> **N**–R)	−19.3 (A119)
Cyclic hydrazine (R_2> NNH_2)	21.7 (A153)
Cyclic tertiary amine-*N*-nitro (R*R*–**N**–(NO_2)–*R*)	−25.7 (A120)
Cyclic tertiary amine-*N*-nitroso (R*R*–**N**–(N=O)–*R*)	−25.7 (A120)
Cyclic secondary amine (R*R*–**NH**–*R*)	2.2 (A121)
Cyclic tertiary amine-*N*-oxide (R*R*–**N**(→**O**)–*R*)	[−22.2] (A122)
Cyclic azoxy group (*R*=**N**(→**O**)–*R*)	[2.9] (A123)
Cyclic secondary amide (*R*–**C**(=**O**)**NH**–*R*)	2.7 (A124)
Cyclic tertiary amide (*R*–**C**(=**O**)**N**< R*R*)	−21.7 (A125)
Cyclic tertiary amide (R–**C**(=**O**)**N**< R_2)	[−9] (A146)
Cyclic carbamate (*R*–**OC**(=**O**)**N**–R*R*)	[−5.2] (A126)
Cyclic carbamate (*R*–**OC**(=**O**)**N**–H*R*)	[19.7] (A154)
Cyclic urea (*R*–**NC**(=**O**)**N**< R*R*)	[−40.6] (A127)
N-Substituted cyclic imide (*R*–**C**(=**O**)**N**(R)**C**(=O)–*R*)	[1.1] (A128)
Cyclic imide (*R*–**C**(=**O**)**N**(**H**)**C**(=**O**)–*R*)	[1.4] (A129)
Cyclic phosphorothioate (*R*–**O**–**P**(=**S**)< (**O**R)(**O***R*))	[−15.6] (A130)
Cyclic phosphazene (=P(X_2))	[−26.7] (A155)
Cyclic sulfide (*R*–**S**–*R*)	2.9 (A131)
Cyclic disulfide (*R*–**SS**–*R*)	[−6.4] (A132)
Cyclic disulfide-*S*-oxide (*R*–**SS**(→**O**)–*R*)	[1.9] (A133)
Cyclic sulphone (*R*–**S**(→**O**)$_2$–*R*)	[−10.4] (A134)
Cyclic thiocarbonate (*R*–**OC**(=**O**)**S**–*R*)	[14.2] (A135)
Cyclic sulfite (*R*–**OS**(→**O**)**O**–*R*)	[−5.8] (A150)
Cyclic thioester (R_1(C=S)SR_2)	[11.0] (A151)
Cyclic sulfate (*R*–**OS**(→**O**)$_2$**O**–*R*)	[0.9] (A136)
Cyclic *N*-substituted sulphonamide (*R*–**S**(→**O**)$_2$**NH**–*R*)	[−0.4] (A137)
Cyclic tertiary sulfonamide ($R_1SO_2NR_2R_3$)	[−27.1] (A152)
Cyclic thiocarbamate (*R*–**S**–(**C**=**O**)**NH***R*)	[13.9] (A138)
Cyclic quaternary silicon (R_2> **Si**< R_2)	−34.7 (A139)

[a] The alphanumerical terms (A1, A2, B2, etc.) are a device used to identify each group value in the estimations provided in Tables 6–8; R: any alkyl or aryl group unless specified otherwise; X: any halogen; values in brackets are tentative assignments; all group coefficients can be assumed to be 1; all group values in this table are to be used with the ring Eq. (2) or (3); values in brackets are tentative assignments.

[b] The R groups that are a part of the ring structure are designated by italics.

in the following functional group contributions: C_2G_{OH} and $3C_2G_F$. Group coefficients for fluorocarbons containing more than three functional groups are not currently available. The group coefficient (C_3) should probably be used whenever more than three different functional groups are present as found previously for other functional groups [9]. The group coefficient C_6 should be used for the CF_2 group contribution only in perfluorinated hydrocarbons. Numerous examples illustrating this protocol can be found in Table 6.

The contributions of the functional groups listed in Table 3 is considerably easier to evaluate. Their contributions are strictly additive and their contributions do not vary with the degree of substitution. These groups are counted as functional groups in molecules containing combinations of functional groups from both Tables 2–5.

2.3. Cyclic and polycyclic compounds

2.3.1. Cyclic and polycyclic hydrocarbons

The total phase change entropy of non-benzenoid cyclic hydrocarbons or benzenoid molecules containing non-benzenoid rings is estimated by using Eq. (2). This equation can be used to estimate $\Delta_0^{T_{fus}}S_{tpce}$ for any parent cycloalkane. The alphanumeric terms (A14 and A15) are used to identify the intercept and slope associated in the estimation of cyclic hydrocarbons. Other terms are defined in Table 4.

$$\Delta S_{ring} = 33.4(A14) + 3.7(A15)(n - 3) \quad (2)$$

where n is the number of ring atoms.

If the cycloalkane contains carbon atoms with a substitution or hybridization pattern that differs from secondary and sp^3, then adjustments to this equation for the appropriate hybridization and substitution pattern for these groups is provided in Table 4. Polycyclic hydrocarbons are modeled using Eq. (3). Adjustments for the bridgehead carbons are obtained from Table 4.

$$\Delta S_{ring} = 33.4(A14)N + 3.7(A15)(R - 3N) \quad (3)$$

where R is the total number of ring atoms and N the number of rings.

The contribution of aliphatic substitutions to either cyclic or polycyclic systems is modeled as described

Narrative continues on pg. 100.

Table 6
Molar transition enthalpies (kJ mol^{-1}) and entropies (J mol^{-1} K^{-1}) of organic and organometallic compounds

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$B_3H_6N_3$ (borazaole)	215.8	Group values are not available	10.61	0	49.17	49.3	10.61	10.6	[185]
$GeBr_4$ (germanium tetrabromide)	299.3	A109 + 4∗A21	12.85	0	42.93	34.8	12.85	10.4	[26]
$GeCl_4$ (germanium tetrachloride)	221.7	4∗A22∗D22 + A102	8.52	0	38.43	29.6	8.52	6.56	[67]
GeF_2 (germanium difluoride)	385.2	Group values are not available	9.25[a]						[159]
GeI_4 (germanium tetraiodide)	419.0	A102 + 4∗A29	19.10	0	45.58	42.4	19.10	17.8	[17]
$N_3P_3Cl_6$ (hexachlorocyclotriphosphazene)	388.6	A14 + 3∗A15 + 6∗A22∗F22 + 3∗A118 + 3∗A155	23.50	0	60.47	63.1	23.50	24.5	[12]
$N_4P_4Cl_8$ (octachlorocyclotetraphosphazene)	400.6	A14 + 5∗A15 + 8∗A22∗F22 + 4∗A118 + 4∗A155	32.20	0	80.38	76.7	32.20	30.73	[12]
SO_3 (γ-sulfur trioxide)	290.2	Group values are not available	9.35	0	32.22	0	9.35	0	[161]
$SiCl_4$ (silicon tetrachloride)	204.7	4∗A22∗D22 + A109	7.72	0	37.72	37.7	7.72	7.7	[160]
CCl_4O_2S (trichloromethanesulfonyl chloride)	227.4	4∗A22∗E22 + A4∗B4 + A157	7.10	31.22					[133]
	418.5		7.46	17.83	49.05	49.0	14.56	20.5	
CH_2O (methanal)	155.0	Group values are not available	7.53	0	48.58		7.53		[132]
CH_4N_2S (thiourea)	169.0	Group values are not available (enthalpy of fusion value is significantly different than value listed immediately below)	0.026	0.15					[22,115]
	200.0		0.113	0.57					
	452.2		12.6	27.86	28.58		12.74		
	169.0		0.026	0.15					[22,188]
	200.0		0.113	0.57					
	444.7		15.64	35.17	35.89		15.78		
$C_2HCl_2F_3$ (1,1,2-trifluoro-1,2-dichloroethane)	135.7	2∗A26∗C26 + A27 + 2∗A22∗E22 + A3∗B3 + A4∗B4	7.08	0	52.16	40.3	7.08	5.5	[42]
$C_2H_2F_3NO$ (trifluoroacetamide)	336.9	A61 + 3∗A25 + A4∗B4	5.58	16.56					[150]
	347.6		11.50	33.08					
	388.9		1.34	3.45	53.09	44.8	18.42	17.3	
$C_2H_2F_4$ (1,1,1,2-tetrafluoroethane)	124.1	3∗A25 + A27 + A4∗B4 + A2	3.62	29.17					[51]
	169.4		2.01	11.87	41.04	36.7	5.63	6.2	
$C_2H_3Cl_3O$ (2,2,2-trichloroethanol)	290.6	A2 + 3∗A22∗D22 + A4∗B4 + A30∗D30	10.05	0	34.58	55.0	10.05	16.0	[37]
$C_2H_4F_2$ (1,1-difluoroethane)	154.6	A1 + 2∗A26 + A3∗B3	1.57	0	10.13	40.6	1.57	6.3	[60]
$C_2H_4N_4$ (dicyandiamide)	269.5	Group values are not available	2.98	11.06					[11]
	487.6		22.96	47.09	58.2		25.94		
C_2H_5NO (*N*-methylformamide)	228.1	A1 + A156	1.23	5.39					[41]
	270.6		10.44	38.58	44.0	44.0	11.7	11.7	
$C_2H_6N_2O_2$ (2-nitro-2-azapropane)	331.5	2∗A1 + A51 + A47	17.26	0	52.06	80.39	17.26	14.2	[35]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_2H_6N_2S$ (1-methyl-2-thiourea)	392.4	A1 + A91	19.46	0	49.59	46.4	19.46	18.2	[188]
C_2H_6Te (dimethyltellurium)	164.1	2∗A1 + A140	0.70	4.26					[28]
	201.9		7.77	38.47	42.73	33.0	8.47	6.7	
$C_3H_2F_6O_2$ (bis-(difluoromethoxy)-difluoromethane)	153.0	6∗A26∗C26 + 2∗A3∗B3 + A4∗B4 + 2∗A32	7.2	0	47.06	50.7	7.2	7.8	[147]
$C_3H_6Cl_2$ (2,2-dichloropropane)	171.6	2∗A22∗B22 + 2∗A1 + A4∗B4	0.01	0.06					[154]
	188.2		0.73	3.89					
	239.6		10.0	41.73	45.69	44.7	10.74	10.7	
C_3H_6O (trimethylene oxide)	173.2	A14 + A15 + A112	6.27	0	36.2	38.3	6.27	6.6	[106]
$C_3H_6O_3$ (methyl glycolate)	272.8	A1 + A2 + A30∗B30 + A38	11.4	0	41.79	50.1	11.4	13.7	[107]
C_3H_7NO (*N*-methylacetamide)	303.7	2∗A1 + A60	10.11	0	33.29	36.70	10.11	11.2	[41]
C_3H_7NO (propanamide)	352.6	A1 + A2 + A61	12.9	0	36.59	52.6	12.9	18.5	[100]
$C_3H_8N_2O_2$ (ethyl carbazate)	318.9	+ A1 + A2 + A69 + A45	20.0	0	62.8	53.8	20.0	17.2	[212]
$C_3H_8N_2S$ (1,3-dimethyl-2-thiourea)	336.9	2∗A1 + A90	12.7	0	37.70	38.4	12.7	12.9	[73]
	337.0		13.71	0	40.68	38.3	13.71	12.9	[188]
$C_3H_8N_2S$ (1-ethyl-2-thiourea)	380.8	A1 + A2 + A91	21.34	0	56.04	53.6	21.34	20.4	[188]
$C_3H_8N_4O_4$ (2,4-dinitro-2,4-diazapentane)	330.2	2∗A1 + A2 + 2∗A51 + 2∗A47	16.36	0	49.55	57.5	16.36	19.0	[35]
$C_4H_2F_8O_2$ (1,2-bis(difluoromethoxy)-1,1,2,2-tetrafluoroethane)	195.0	8∗A26∗C26 + 2∗A3∗B3 + 2∗A4∗B4 + 2∗A32	11.8	0	60.5	55.7	11.8	10.9	[147]
$C_4H_2F_8O_3$ (oxybis[(difluoromethoxy)-difluoromethane])	153.0	8∗A26∗C26 + 2∗A3∗B3 + 2∗A4∗B4 + 3∗A32	3.1	0	20.26	60.5	3.1	9.2	[147]
$C_4H_6N_4O_4$ (2,5-dinitro-2,5-diazahexane-3,4-dione)	397.1	2∗A1 + A2 + 2∗A51 + 2∗A35 + 2∗A47	23.40	0	58.93	92.4	23.40	36.7	[35]
C_4H_6Te (divinyltellurium)	182.6	2∗A6∗B6 + 2∗A5 + A140	9.59	0	52.52	40.4	9.59	7.4	[32]
$C_4H_7NO_2$ ((−) 4-hydroxy-2-pyrrolidone)	429.8	A14 + 2∗A15 + A124 + A30∗B30 + A16	28.49	0	66.29	46.6	28.49	20.0	[71]
$C_4H_7NO_2$ ((±) 4-hydroxy-2-pyrrolidone)	394.8	A14 + 2∗A15 + A124 + A30∗B30 + A16	26.74	0	67.73	46.6	26.74	18.4	[71]
$C_4H_8N_2O_7$ (diethylene glycol dinitrate)	276.5	4∗A2 + A32 + 2∗A55	25.4	0	91.9	81.9	25.4	22.6	[215]
$C_4H_8N_4O_4$ (1,4-dinitro-1,4-diazacyclohexane)	489.6	A14 + 3∗A15 + 2∗A120 + 2∗A51	33.93	0	69.30	63.3	33.93	31.0	[35]
$C_4H_8N_6O_6$ (1,3,5-trinitro-1,3,5-triazacycloheptane)	435.9	A14 + 4∗A15 + 3∗A120 + 3∗A51	27.74	0	63.63	74.6	27.74	33.3	[35]
C_4H_8O (cyclobutanol)	228.4	A14 + A15 + A16 + A30	8.53	0	37.34	24.1	8.53	5.50	[65]
$C_4H_8O_2S$ (sulfolane)	288.6		7.86	27.34					
	301.7	A14 + 2∗A15 + A134	1.37	4.54	31.88	30.4	9.23	9.2	[41]
$C_4H_9Cl_3Si$ (trichloromethyltrimethylsilane)	285.5	3∗A1 + A4∗B4 + 3∗A22∗D22 + A109	11.16	39.09					[21]

	405.3		7.36	18.16	57.25	51.3	18.52	20.8	
$C_4H_9Cl_3Si$ (*tert*-butyltrichlorosilane)	206.4	3∗A1 + A4∗B4 + 3∗A22∗D22 + A109	6.01	29.12					[21]
	373.4		6.69	17.92	47.04	51.3	12.70	19.2	
C_4H_9NO (*N*,*N*-dimethylacetamide)	251.4	3∗A1 + A59	10.42	0	41.44	41.6	10.42	10.5	[41]
	253.2		8.2	0	32.4	41.6	8.2	10.5	[209]
C_4H_9NO (butanamide)	387.3	A1 + 2∗A2 + A61	19.2	0	49.57	64.1	19.2	24.8	[102]
$C_4H_9NO_2$ (2-methyl-2-nitropropane)	215.3	3∗A1 + A50 + A3∗B3	4.2	19.51					[141]
	260.1		4.7	18.07					
	299.2		2.6	8.69	46.27	60.7	11.5	18.2	
$C_4H_9NO_3$ (2-methyl-2-nitro-1-propanol)	311.5	2∗A1 + A4∗B4 + A30∗B30 + A50	14.64	47.00					[142]
	363.9		3.17	8.71	55.71	55.3	17.81	20.1	
$C_4H_{10}N_2$ (piperazine)	384.6	A14 + 3∗A15 + 2∗A121	26.7	0	69.42	48.9	26.7	18.8	[124]
$C_4H_{10}N_6O_6$ (2,4,6-trinitro-2,4,6-triazaheptane)	442.4	2∗A1 + 2∗A2 + 3∗A51 + 3∗A47	34.01	0	76.88	72.2	34.01	31.9	[35]
$C_4H_{12}S_4Ge$ (tetra(methylthia)germane)	284.1	4∗A1 + 4∗A84 + A102	14.2	0	49.98	43.6	14.2	12.4	[82]
$C_4H_{12}S_4Si$ (tetra(methylthia)silane)	288.6	4∗A1 + 4∗A84 + A109	11.63	40.30					[82]
	304.5		2.18	7.16	47.46	51.7	13.81	15.7	
$C_4H_{12}S_4Sn$ (tetra(methylthia)tin)	307.5	4∗A1 + 4∗A84 + A110	24.1	0	78.37	54.6	24.1	16.8	[82]
$C_5H_3N_3$ (2,2-dicyanopropanionitrile)	367.2	A1 + 3∗A56 + A4∗B4	18.70	0	50.93	47.7	18.70	17.5	[74]
$C_5H_4N_4$ (1,2,4-trazolo[1,5a]pyrimidine)	419.5	Group values are not available	19.4	0	46.25		19.4		[124]
$C_5H_5N_3O$ (pyrazinecarboxamide)	463.0	3∗A10 + A12 + 2∗A41 + A61	30.28	0	65.40	64.4	30.28	29.8	[172]
$C_5H_6N_2$ (2-aminopyridine)	331.5	4∗A10 + A12 + A41 + A45	15.3	0	46.15	54.5	15.3	18.1	[43]
$C_5H_6N_2$ (3-aminopyridine)	335.5	4∗A10 + A12 + A41 + A45	14.4	0	42.92	54.5	14.4	18.3	[43]
$C_5H_7Cl_3O_2$ (3-chloro-2, 2-bis(chloromethyl)propionic acid)	383.9	3∗A2 + A4∗B4 + 3∗A22∗D22 + A36∗D36	20.9	0	54.2	77.1	20.9	29.6	[81]
$C_5H_7N_3O_5$ (*N*-acetyl-3, 3-dinitroazetidine)	386.9	A14 + A15 + A1 + A146 + 2∗A50 + A17	25.65	0	66.30	46.5	25.65	18.0	[138]
$C_5H_9ClO_2$ (*n*-propyl chloroacetate)	110.0	A1 + 3∗A2 + A22∗B22 + A38	0.36	3.27					[89]
	204.0		0.69	3.38					
	207.0		0.17	0.82					
	240.0		13.0	54.17	61.64	62.8	14.22	15.1	
$C_5H_9Cl_3$ (2-chloromethyl-2-methyl-1, 3-dichloropropane)	246.6	A1 + 3∗A2 + 3∗A22∗C22 + A4	12.0	48.66					[79]
	291.3		2.5	8.58	57.24	52.7	14.5	15.4	
C_5H_9NO (*N*-methylpyrrolidinone)	248.5	A14 + 2∗A15 + A125 + A1	18.1	0	72.8	36.7	18.1	9.1	[209]
$C_5H_{10}Br_2O_2$ (2,2-bis(bromomethyl)-1, 3-propanediol)	387.3	4∗A2 + 2∗A30∗D30 + 2∗A21 + A4	30.1	0	77.72	73.1	30.1	28.3	[79]
$C_5H_{10}Cl_2$ (1,3-dichloro-2, 2-dimethylpropane)	193.8	2∗A1 + A4 + 2∗A2 + 2∗A22∗B22	0.6	3.2					[81]
	198.4		3.6	17.9					
	262.2		1.6	6.0	27.1	47.0	5.8	12.3	
$C_5H_{10}O$ (pentanal)	151.6	A1 + 3∗A2∗B2 + A34	15.0	0	98.94	67.0	15.0	10.2	[132]
$C_5H_{12}N_2S$ (1,3-diethyl-2-thiourea)	350.5	2∗A1 + 2∗A2 + A90	17.14	0	48.90	52.6	17.14	18.4	[188]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_5H_{12}N_2S$ (1,1,3,3-tetramethyl-2-thiourea)	350.4	4∗A1 + A148	22.14	0	63.18	63.2	22.14	22.1	[188]
$C_5H_{12}O$ (2,2-dimethyl-1-propanol)	235.4	3∗A1 + A4 + A2 + A30	4.14	17.59					[142]
	329.8		3.73	11.30	28.90	26.8	7.87	8.8	
$C_5H_{12}O_2$ (2,2-dimethyl-1, 3-propanediol)	60.4	2∗A1 + 2∗A2 + A4 + 2∗A30∗B30	0.18	2.93					[142]
	314.4		12.43	39.54					
	402.8		4.34	10.77	53.3	49.9	16.95	20.1	
$C_5H_{12}O_3$ (2-hydroxymethyl-2-methyl-1,3-propanediol)	356.7	A1 + 3∗A2 + A4 + 3∗A30∗C30	20.94	58.70					[142]
	474.4		4.72	9.95	68.65	53.6	25.66	25.4	
$C_5H_{13}NSi$ (trimethylsilylethyleneimine)	192.5	3∗A1 + A14 + A119 + A109	10.50	0	54.5	39.8	10.50	7.7	[103]
$C_5H_{14}N_2$ (2,2-dimethyl-1, 3-diaminopropane)	194.2	2∗A1 + 2∗A2 + A4 + 2∗A45	14.7	75.70					[80]
	301.7		1.7	5.63	81.33	57.4	16.4	17.3	
$C_6D_{10}O$ (cyclohexanone-d_{10})	216.8	A14 + 3∗A15 + A114	7.10	32.74					[39]
	219.3		0.40	1.82					
	241.5		1.19	4.93	39.49	43.1	8.69	10.4	
C_6H_4ClI (1-chloro-4-iodobenzene)	326.7	4∗A10 + 2∗A12 + A29 + A22∗B22	16.10	0	49.28	50.2	16.10	16.4	[152]
$C_6H_5N_3$ (1*H*-benzotriazole)	369.9	A14 + 2∗A15 + 2∗A19 + 4∗A10 + A121 + 2∗A118	7.70	0	20.82	49.0	7.70	18.1	[30]
C_6H_6BrN (2-bromoaniline)	305.0	4∗A10 + A45 + A21 + 2∗A12	20.04	0	65.71	53.5	20.04	16.3	[66]
C_6H_6BrN (3-bromoaniline)	291.0	4∗A10 + A45 + A21 + 2∗A12	14.68	0	50.45	53.5	14.7	15.6	[66]
C_6H_6BrN (4-bromoaniline)	336.0	4∗A10 + A45 + A21 + 2∗A12	13.36	0	39.76	53.5	14.36	18.0	[66]
C_6H_6ClN (2-chloroaniline)	271.0	4∗A10 + A45 + A22∗B22 + 2∗A12	8.81	0	32.51	52.2	8.81	14.2	[66]
C_6H_6ClN (3-chloroaniline)	263.0	4∗A10 + A45 + A22∗B22 + 2∗A12	12.00	0	45.63	52.2	12.00	13.7	[66]
C_6H_6ClN (4-chloroaniline)	344.0	4∗A10 + A45 + A22∗B22 + 2∗A12	16.90	0	49.13	52.2	16.90	18.0	[66]
C_6H_6IN (2-iodoaniline)	333.0	4∗A10 + A45 + A29 + 2∗A12	13.95	0	41.89	55.4	13.95	18.4	[66]
C_6H_6IN (3-iodoaniline)	298.0	4∗A10 + A45 + A29 + 2∗A12	14.50	0	48.66	55.4	14.50	16.5	[66]
C_6H_6IN (4-iodoaniline)	334.0	4∗A10 + A45 + A29 + 2∗A12	15.10	0	45.21	55.4	15.10	18.5	[66]
$C_6H_6N_2O$ (picolinamide)	381.0	4∗A10 + A12 + A41 + A61	16.82	0	44.15	60.9	16.82	23.2	[172]
$C_6H_6N_2O$ (isonicotinamide)	431.0	4∗A10 + A12 + A41 + A61	26.81	0	62.2	60.9	26.81	26.3	[172]
$C_6H_6N_2O$ (nicotinamide)	402.0	4∗A10 + A12 + A41 + A61	26.94	0	67.01	60.9	26.94	24.5	[172]

$C_6H_6O_2$ (1,2-dihydroxybenzene)	377.6	4∗A10 + 2∗A31 + 2∗A12	18.55	0	49.13	55.2	18.55	20.8	[179]
$C_6H_8N_2O_8$ (1,4:3,6-dianhydromannitol dinitrate (isomannide dinitrate))	337.2	2∗A14 + 2∗A15 + 2∗A112 + 4∗A16 + 2∗A55	20.50	0	60.79	66.6	20.50	22.5	[164][b]
$C_6H_8N_2O_8$ (1,4:3,6-dianhydro-D-glucitol dinitrate (isosorbide dinitrate))	341.7	2∗A14 + 2∗A15 + 2∗A112 + 4∗A16 + 2∗A55	27.63	0	80.86	66.6	27.63	22.8	[164][b]
$C_6H_8N_2O_8$ (1,4:3,6-dianhydroiditol dinitrate (isoidide dinitrate))	325.9	2∗A14 + 2∗A15 + 2∗A112 + 4∗A16 + 2∗A55	12.81	0	39.31	66.6	12.81	21.7	[164][b]
$C_6H_8N_6O_8$ (1,3-dinitro-3(1′,3′-dinitroazetidin-3′-yl)azetidine)	387.5	2∗A14 + 2∗A15 + 2∗A17 + 2∗A51 + 2∗A120 + 2∗A50	25.52	0	65.86	65.8	25.52	25.5	[111]
$C_6H_8O_4$ (L-3,6-dimethyl-1, 4-dioxane-2,5-dione)	366.6	A14 + A15 + 2∗A115 + 2∗A16 + 2∗A1	16.94	0	46.2	49.1	16.94	18.0	[33]
$C_6H_9NO_6$ (isomannide mononitrate)	344.8	2∗A14 + 2∗A15 + 2∗A112 + 4∗A16 + A55 + A30∗D30	20.64	0	59.86	64.5	20.64	22.2	[164][b]
$C_6H_9NO_6$ (isosorbide-2-mononitrate)	328.0	2∗A14 + 2∗A15 + 2∗A112 + 4∗A16 + A55 + A30∗D30	26.38	0	80.43	64.5	26.38	21.2	[164][b]
$C_6H_9NO_6$ (isosorbide-5-mononitrate)	364.0	2∗A14 + 2∗A15 + 2∗A112 + 4∗A16 + A55 + A30∗D30	22.36	0	61.43	64.5	22.36	23.5	[164][b]
$C_6H_{10}Cl_2$ (1,1-dichlorocyclohexane)	225.0	A14 + 3∗A15 + 2∗A22∗B22	9.16	40.71					[176]
	236.6		1.47	6.21	46.92	42.3	10.63	10.0	
$C_6H_{10}O$ (7-oxabicyclo[2.2.1]heptane)	180.5	2∗A14 + A15 + 2∗A16 + A112	4.86	26.9					[91][c]
	218.5		0.98	4.5					
	244.0		0.71	2.6	34.0	42.3	6.55	10.3	
$C_6H_{10}O_3$ (4-methyl-2,6, 7-trioxabicyclo[2.2.2]octane)	369.2	2∗A14 + 2∗A15 + 3∗A112 + A1 + A17 + A16	10.4	0	28.17	46.1	10.4	17.0	[86]
$C_6H_{10}O_4$ (*trans*-1,3,5,7-tetraoxadecalin)	374.5	2∗A14 + 4∗A15 + 2∗A16 + 4∗A112	23.14	0	61.78	57.0	23.14	21.4	[78]
$C_6H_{10}O_4$ (*cis*-1,3,5,7-tetraoxadecalin)	450.2	2∗A14 + 4∗A15 + 2∗A16 + 4∗A112	28.62	0	63.57	57.0	28.62	25.7	[78]
$C_6H_{10}O_5$ (1,6-anhydro-β-D-gulopyranose)	404.0	2∗A14 + 2∗A15 + 5∗A16 + 3∗A30∗E30 + 2∗A112	24.5	0	60.6	64.8	24.5	26.2	[167]
$C_6H_{11}F$ (fluorocyclohexane)	186.7	A14 + 3∗A15 + A16 + A28	7.82	41.89					[19]
	285.3		2.58	9.04	50.93	47.3	10.40	13.5	
$C_6H_{12}N_2O$ (1,4-diazabicyclo-[2.2.2]octane-*N*-oxide)	418.0	2∗A14 + 2∗A15 + A119 + A122	3.4	8.14					[57]
	493.0		0.45	0.91	9.05	32.7	3.85	16.1	
$C_6H_{12}Si$ (1,1-dimethyl-1-silacyclopent-3-ene)	166.8	A14 + 2∗A15 + 2∗A18 + 2∗A1 + A139	7.77	0	46.58	38.1	7.77	6.4	[173][d]
$C_6H_{13}N$ (aminocyclohexane)	258.2	A14 + 3∗A15 + A16 + A45	1.00	3.96					[38]
	255.1		16.5	64.68	68.64	51.2	17.5	13.1	
	255.4		14.92	0	58.42	51.2	14.92	13.1	[175,176]
$C_6H_{14}N_8O_8$ (2,4,7,9-tetranitro-2, 4,7,9-tetraazadecane)	488.1	2∗A1 + 4∗A2 + 4∗A51 + 4∗A47	68.09	0	139.5	94.0	68.09	45.9	[35]
$C_6H_{14}O_2$ (2-butoxyethanol)	199.5	A1 + 5∗A2 + A30∗B30 + A32	11.8	0	59.15	75.5	11.8	15.1	[187]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_6H_{14}O_2$ (2-*tert*-butoxyethanol)	223.1	3∗A1 + A4∗B4 + 2∗A2 + A30∗B30 + A32	11.4	0	51.10	66.4	11.4	14.9	[187]
$C_6H_{15}ClSi$ (*tert*-butyldimethylchlorosilane)	203.6	5∗A1 + A4∗B4 + A22∗B22 + A109	7.75	38.06					[21]
	358.1		5.60	15.64	53.70	54.1	13.35	19.4	
$C_6H_{15}P$ (triethylphosphine)	188.2	3∗A1 + 3∗A2 + A72	10.73	0	57.04	53.4	10.73	10.1	[48]
$C_6H_{16}N_2$ (*N*,*N*-bis-(2-hydroxyethyl)-ethylenediamine)	373.2	6∗A2 + 2∗A44 + 2∗A30∗D30	49.7	0	133.2	76.5	49.7	28.6	[124]
$C_7H_5FO_2$ (4-fluorobenzoic acid)	451.2	4∗A10 + 2∗A12 + A24 + A36∗B36	20.9	0	46.32	47.41	20.9	21.4	[121]
$C_7H_6INO_2$ (3-iodo-2-nitrotoluene)	339.3	3∗A10 + A11 + 2∗A12 + A1 + A29 + A50	20.68	0	60.9	52.3	20.7	17.7	[206,214]
$C_7H_7BCl_2$ (*p*-tolyldichloroborane)	301.0	Group values are not available	4.39	0	14.58		4.39		[54]
$C_7H_7ClN_2O$ (2-chlorobenzoic acid hydrazide)	392.2	4∗A10 + 2∗A12 + A147 + 2∗A22∗B22	25.6	0	65.2	74.3	25.6	29.1	This work
$C_7H_7ClN_2O$ (4-chlorobenzoic acid hydrazide)	437.2	4∗A10 + 2∗A12 + A147 + 2∗A22∗B22	32.9	0	75.2	74.3	32.9	32.5	This work
C_7H_8 (bicyclo[2.2.1]hept-2,5-diene)	202.0	Fusion values not reported	8.93	44.2					[123]
$C_7H_8ClN_3O_4S_2$ (6-chloro-3,4-dihydro-2*H*-1,2,4-benzothiadiazine-7-sulfonamide-1,1-dioxide (hydrochlorthiazide))	547.2	A14 + 3∗A15 + A137 + 2∗A12 + 2∗A10 + A96 + A22∗D22 + A121 + 2∗A19	30.96	0	56.58	66.1	30.96	36.2	[183]
$C_7H_8N_2O$ (*N*-(2-pyridyl)acetamide)	343.0	4∗A10 + A1 + A60 + A41 + A12	16.0	0	46.64	52.1	16.0	17.9	[157]
$C_7H_8N_2O$ (benzoic acid hydrazide)	388.2	5∗A10 + A12 + A147	25.7	0	66.2	56.8	25.7	22.0	This work
$C_7H_8O_2$ (2-methyl-1, 4-dihydroxybenzene)	404.2	A1 + 3∗A10 + A11 + 2∗A12 + 2∗A31	27.60	0	68.28	55.8	27.60	22.6	[50]
$C_7H_{10}O_6$ (tri(methoxycarbonyl)methane)	301.2	3∗A1 + 3∗A38 + A3∗B3	18.2	0	60.42	66.1	18.2	19.9	[85]
$C_7H_{12}N_2$ (2-piperidinoacetonitrile)	293.2	A14 + 3∗A15 + A56 + A2 + A119	17.57	0	59.92	50.0	17.57	14.7	[87]
$C_7H_{12}O_2$ (cyclohexylformate)	201.3	A14 + 3∗A15 + A16 + A37	10.49	0	52.11	53.6	10.49	10.8	[176]
$C_7H_{12}O_3$ (1,4-dimethyl-2,6, 7-trioxabicyclo[2.2.2]octane)	370.2	2∗A14 + 2∗A15 + 3∗A112 + 2∗A1 + 2∗A17	18.0	0	48.62	43.8	18.0	16.2	[86]
$C_7H_{13}Cl$ (1-chloro-1-methylcyclohexane)	214.4		9.38	43.76					
	234.5	A14 + 3∗A15 + A1 + A17 + A22	1.63	6.95	50.71	38.3	11.01	9.0	[27]
$C_7H_{14}O$ (1-methylcyclohexanol)	299.4	A14 + 3∗A15 + A1 + A17 + A30	14.32	0	47.83	29.2	14.32	8.7	[27]

$C_7H_{14}O_6$ (methyl-α-D-glucopyranoside)	436.0	A14 + 3∗A15 + A1 + A2 + A32 + A112 + 4∗A30∗E30 + 5∗A16	35.11	0	80.53	90.7	35.11	39.5	[170]
$C_7H_{14}O_6$ (methyl-β-D-glucopyranoside)	384.9	A14 + 3∗A15 + A1 + A2 + A32 + A112 + 4∗A30∗E30 + 5∗A16	27.03	0	70.23	83.9	27.03	32.3	[170]
$C_7H_{14}O_6$ (methyl-α-D-galactopyranoside)	397.6	A14 + 3∗A15 + A1 + A2 + A32 + A112 + 4∗A30∗E30 + 5∗A16	27.95	0	70.30	83.9	27.95	33.4	[170]
$C_7H_{14}O_6$ (methyl-β-D-galactopyranoside)	450.9	A14 + 3∗A15 + A1 + A2 + A32 + A112 + 4∗A30∗E30 + 5∗A16	33.18	0	73.59	83.9	33.18	37.8	[170]
$C_7H_{15}NO_4$ (*N*-methyl-5-amino-1, 5-dideoxy-D-glycopyranose)	425.7	A14 + 3∗A15 + 4∗A16 + A119 + 4∗A30∗E30 + A1 + A2	27.5	0	64.60	73.4	27.5	31.2	[25]
$C_8H_{17}NO_4$ (*N*-ethyl-5-amino-1, 5-dideoxy-D-glycopyranose)	429.1	A14 + 3∗A15 + 4∗A16 + A119 + 4∗A30∗E30 + A1 + A2	26.30	0	61.29	73.38	26.30	31.5	[25]
$C_7H_{16}N_2O$ (*n*-hexyl urea)	380.2	A1 + 5∗A2∗B2 + A67	26.5	0	69.70	81.0	26.5	30.8	[145]
$C_7H_{16}N_2S$ (1,3-dipropyl-2-thiourea)	342.6	2∗A1 + 4∗A2 + A90	22.90	0	66.84	66.8	22.90	22.9	[188]
$C_8H_2C_4N_2$ (2,3,6, 7-tetrachloroquinoxaline)	446	2∗A10 + 6∗A12 + 2∗A41 + 4∗A22∗F22	29.6	0	66.4	56.4	26.9	25.2	[213]
$C_8H_4Cl_2N_2$ (2,3-dichloroquinoxaline)	424.4	4∗A10 + 4∗A12 + 2∗A41 + 2∗A22∗D22	24.36	0	57.40	53.8	24.36	22.8	[213]
$C_8H_6N_2O$ (2-hydroxyquinoxaline)	542.5	5∗A10 + 3∗A12 + 2∗A41 + A31	32.5	0	59.8	56.6	32.5	30.7	[213]
$C_8H_6O_2$ (phthalic acid)	463.5	4∗A10 + 2∗A12 + 2∗A36∗B36	36.5	0	78.75	47.0	36.5	21.8	[46]
$C_8H_6O_2$ (isophthalic acid)	617.4	4∗A10 + 2∗A12 + 2∗A36∗B36	43.2	0	69.97	47.03	43.2	29.0	[46]
$C_8H_7ClO_3$ (5-chloro-4-hydroxy-3-methoxybenzaldehyde)	442.6	2∗A10 + 4∗A12 + A22∗D22 + A31 + A1 + A34 + A32	39.4	0	89.02	65.11	39.4	28.8	[101]
$C_8H_8O_2$ (methyl benzoate)	260.8	5∗A10 + A12 + A1 + A38	14.83	0	56.86	54.8	14.83	14.3	[83]
$C_8H_{12}BrN_5O_3$ (8-bromo-9-[(2-hydroxyethoxy)methyl]quanine)	452.9	2∗A14 + 3∗A15 + 3∗A2 + A32 + A45 + 4∗A19 + A21 + A119 + 2∗A118 + A124 + A30∗E30	36.44	0	80.47	100.3	36.44	45.4	[31]
$C_8H_{14}O_2$ (*n*-butylmethacrylate)	197.8	2∗A1 + 3∗A2 + A5 + A7 + A38	15.55	0	78.62	70.8	15.55	14.0	[44]
$C_8H_{14}O_2$ (cyclohexyl acetate)	221.8		5.23	23.58					
	224.6	A14 + 3∗A15 + A16 + A1 + A38	8.00	35.62	59.20	55.1	13.23	12.4	[176]
$C_8H_{14}O_6S$ (dimethyl-3, 3′-sulfonyldipropionate)	390.3	2∗A1 + 4∗A2 + 2∗A38 + A88	41.1	0	105.3	79.3	41.1	31.0	[62]
$C_8D_{14}O_2$ (*n*-perdeuteriobutylmethacrylate)	198.1	2∗A1 + 3∗A2 + A5 + A7 + A38	16.04	0	81.00	70.8	16.04	14.0	[44]
$C_8H_{18}B_{10}O_3$ (1,2-dicarbadodecaborane(12)-1-carboperoxoic acid, 1,1-dimethyl-2-propynyl ester)	374.0	Group values are not available	16.0	0	42.78		16.0		[104]
$C_8H_{18}B_{10}O_3$ (1,7-dicarbadodecaborane(12)-1-carboperoxoic acid, 1, 1-dimethyl-2-propynyl ester)	360.0	Group values are not available	29.4	0	81.67		29.4		[104]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_8H_{18}N_2O$ (*n*-heptyl urea)	379.2		1.4	3.69					
	382.2	A1 + 6∗A2∗B2 + A67	26.3	68.81	72.50	90.3	27.7	34.5	[145]
C_9F_{16} (*cis*-perfluorobicyclo-[4.3.0]nonane)	200.6	2∗A14 + 3∗A15 + 16∗A28 + 9∗A17	8.76	43.67					[10]
	245.6		1.27	5.17					
	291.3		2.72	9.34	58.18	46.5	12.75	13.5	
C_9F_{16} (*trans*-perfluorobicyclo-[4.3.0]nonane)	236.6	2∗A14 + 3∗A15 + 16∗A28 + 9∗A17	8.91	37.66					[10]
	248.1		2.63	10.60	48.26	46.5	11.54	11.5	
$C_9H_6Cl_6O_3S$ (6,7,8,9,10, 10-hexachloro-1,5,5a,6,9, 9a-hexahydro-6,9-methano-2,4, 3-benzodioxathiepin-3-oxide (endosulfan))	368.0	3∗A14 + 3∗A15 + 6∗A22∗F22 + 3∗A17 + 2∗A19 + 2∗A16 + A150	16.52	0	44.89	44.9	16.52	16.5	[174]
$C_9H_6S_3$ (5-phenyldithiolethione)	398.0	A14 + 2∗A15 + 5∗A10 + A12 + A18 + A19 + A132 + A151	26.27	0	66.01	61.0	26.27	24.3	[68]
$C_9H_8N_2O$ (2-hydroxy-3-methylquinoxaline)	522.9	4∗A10 + 3∗A12 + A11 + A1 + 2∗A41 + A31	33.4	0	63.9	57.2	33.4	29.9	[215]
C_9H_8O (1-indanone)	312.9	A14 + 2∗A15 + 4∗A10 + 2∗A19 + A114	17.78	0	56.82	44.4	17.78	13.9	[14]
$C_9H_8O_4$ (2-acetoxybenzoic acid)	414.0	A1 + A38 + A36∗B36 + 4∗A10 + 2∗A12	29.80	0	71.98	56.1	29.80	23.2	[166]
C_9H_9N (2-methylindole)	329.4	A1 + 4∗A10 + A14 + 2∗A15 + A18 + 3∗A19 + A121	15.72	0	47.72	51.7	15.72	17.0	[116]
$C_9H_{10}N_2$ (*N*-amino-2-methylindole)	384.6	A1 + 4∗A10 + A14 + 2∗A15 + A18 + 3∗A19 + A121	25.55	0	66.43	71.2	25.55	27.4	[116]
$C_9H_{10}O_2$ (methyl *o*-toluate)	228.8	4∗A10 + A12 + A11 + 2∗A1 + A38	12.50	0	54.84	55.4	12.50	12.68	[83]
$C_9H_{10}O_2$ (methyl *m*-toluate)	269.9	4∗A10 + A12 + A11 + 2∗A1 + A38	21.15	0	79.66	55.4	21.15	14.95	[83]
$C_9H_{10}O_2$ (methyl *p*-toluate)	306.5	4∗A10 + A12 + A11 + 2∗A1 + A38	20.77	0	67.77	55.4	20.77	16.98	[83]
$C_9H_{11}NO$ (4-dimethylamino-benzaldehyde)	346.2	4∗A10 + 2∗A12 + 2∗A1 + A34 + A43	19.07	0	55.08	49.10	19.07	17.00	[64]
C_9H_{12} (1,3,5-trimethylbenzene)	91.3	3∗A1 + 3∗A10 + 3∗A11	0.33	3.6					[210]
	188.5		0.07	0.4					
	228.4		9.51	41.7	45.7	46.2	9.9	10.6	[158]
$C_9H_{12}N_2$ (*N*-amino-2-methylindoline)	318.2	+ A1 + 4∗A10 + A14 + 2∗A15 A18 + 3∗A19 + A153	24.45	0	76.84	71.2	24.45	22.4	[116]

$C_9H_{12}N_2O_2S_2$ (*S*-methyl-*N*′-tosylisothiourea)	401.2	2∗A1 + 4∗A10 + A11 + A12 + A160	31.20	0	77.77	77.8	31.20	31.2	[23]
$C_9H_{12}O$ (2,3,6-trimethylphenol)	331.2	3∗A1 + A31 + 2∗A10 + 3∗A11 + A12	22.05	0	66.57	51.60	22.05	17.1	[63]
$C_9H_{13}NO$ ((−) 2-amino-1-phenyl-1-propanol (norephedrine))	324.4	5∗A10 + A1 + 2∗A3∗B3 + A30∗B30 + A45 + A11	15.87	0	48.92	64.4	15.87	20.9	[71]
$C_9H_{13}NO$ ((±) 2-amino-1-phenyl-1-propanol (norephedrine))	374.3	5∗A10 + A1 + 2∗A3∗B3 + A30∗B30 + A45 + A11	26.11	0	69.76	64.4	26.11	24.10	[71]
$C_9H_{13}N_5O_4$ (9-[(1,3-dihydroxy-2-propoxy)methyl]quanine)	509.2	2∗A14 + 3∗A15 + 3∗A2 + A32 + A45 + 3∗A19 + A18∗B18 + A119 + 2∗A118 + A124 + 2∗A30∗E30 + A3∗B3	37.88	0	74.39	104.4	37.88	53.2	[31]
$C_9H_{16}N_2$ (2-methyl-2-piperidinopropionitrile)	316.2	2∗A1 + A14 + 3∗A15 + A4∗B4 + A56 + A119	21.59	0	68.28	55.1	21.59	17.4	[87]
$C_9H_{16}O_3$ (4-methyl-1-propyl-2,6,7-trioxabicyclo[2.2.2]octane)	311.2	2∗A14 + 2∗A15 + 3∗A112 + 2∗A1 + 2∗A2 + 2∗A17	16.1	0	51.75	58.0	16.1	18.0	[86]
C_9H_{20} (2-methyloctane)	192.8	3∗A1 + A3 + 5∗A2∗B2	17.99	0	93.31	82.9	17.99	16.0	[70]
C_9H_{20} (3-methyloctane)	165.6	3∗A1 + A3 + A2 + 4∗A2∗B2	16.99	0	102.6	80.7	16.99	13.4	[70]
$C_9H_{20}N_2O$ (*n*-octyl urea)	350.2		11.5	32.84					
	372.2	A1 + 7∗A2∗B2 + A67	24.6	66.09	98.93	99.6	36.1	37.1	[145]
$C_9H_{20}N_2S$ (1,3-dibutyl-2-thiourea)	338.0	2∗A1 + A90 + 6∗A2∗B2	28.34	0	83.85	94.1	28.34	31.8	[188]
$C_9H_{20}O_4$ (3,3′-[1,3-propanediylbis(oxy)]bis-1-propanol)	263.1	9∗A2∗B2 + 2∗A32 + 2∗A30∗E30	21.15	0	80.39	117.9	21.15	31.1	[109]
$C_9H_{27}NSi_3$ (tris(trimethylsilyl)amine)	244.2		7.90	32.35					
	337.2	9∗A1 + 3∗A109 + A43	1.77	5.25	37.6	54.9	9.67	18.5	[108]
$C_{10}F_8$ (octafluoronaphthalene)	283.6		2.12	7.48					
	358.8	10∗A12 + 8∗A24	17.55	48.91	56.39	57.8	19.67	20.7	[153]
$C_{10}H_5Cl_7$ (1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-endomethanoindene (heptachlor))	362.2	3∗A14 + A15 + 3∗A17 + 2∗A19 + 7∗A22∗F22 + 2∗A18 + 3A16	20.72	0	57.21	41.6	20.72	15.1	[174]
$C_{10}H_8Br_2N_2$ (2,3-bis(bromomethyl)quinoxaline)	423.6	4∗A10 + 2∗A12 + 2∗A11 + 2∗A41 + 2∗A2 + 2∗A21	32.43	0	76.6	66.4	32.4	28.1	[213]
$C_{10}H_8Cl_2O_6$ (3,6-dichloro-2,5-dihydroxyterephthalate)	380.0		1.7	4.5					
	455.0	6∗A12 + 2∗A1 + 2∗A38 + 2∗A31 + 2∗A22∗F22	41.0	90.1	94.6	78.6	42.7	35.8	[130]
$C_{10}H_8OS_3$ (5-(4-methoxyphenyl)-3*H*-1,2-dithiole-3-thione)	382.2	A14 + 2∗A15 + A1 + 4∗A10 + 2∗A12 + A32 + A18 + A19 + A132 + A151	24.39	0	63.81	68.6	24.39	26.2	[68]
$C_{10}H_9Br$ (bromobullvalene)	317.2	3∗A14 + A15 + 4∗A16 + 5∗A18 + A21 + A19	14.20	0	44.77	42.3	14.20	13.7	[18]
$C_{10}H_9Cl$ (chlorobullvalene)	287.2	3∗A14 + A15 + 4∗A16 + 5∗A18 + A22 + A19	13.50	0	47.01	35.6	13.50	10.2	[18]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{10}H_9I$ (iodobullvalene)	376.2	3∗A14 + A15 + 4∗A16 + 5∗A18 + A29 + A19	15.50	0	41.20	44.2	15.50	16.6	[18]
$C_{10}H_{10}$ (1,4-dihydronaphthalene)	298.1	A14 + 3∗A15 + 4∗A10 + 2∗A19 + 2∗A18	9.35	0	31.37	46.3	9.35	13.8	[34]
$C_{10}H_{10}Fe$ (ferrocene)	163.9	Group values are not available	0.90	5.49					[52,53]
	242.0		4.14	17.11					
	448.2		17.78	39.67	62.27		22.82		
$C_{10}H_{10}N_2$ (2,3-dimethylquinoxaline)	379.5	4∗A10 + 2∗A12 + 2∗A11 + 2∗A41 + 2∗A1	22.35	0	58.9	52.4	22.3	19.9	[213]
$C_{10}H_{10}N_2O_5$ (2,3-dihydro-3-[2-(nitrooxy)ethyl]-4*H*-1,3-benzoxazin-4-one)	326.3	A14 + 3∗A15 + 2∗A2 + A125 + A112 + 2∗A19 + 4∗A10 + A55	23.0	0	70.50	67.6	23.0	22.1	[165]
$C_{10}H_{10}N_4O_2S$ (4-amino-*N*-(2-pyrmidinyl)benzene sulfonamide (sulfadiazine))	520.4	7∗A10 + 3∗A12 + 4∗A41 + A95 + A45	44.3	0	85.13	78.8	44.3	41.0	[181]
$C_{10}H_{10}O_4$ (dimethyl phthalate)	274.2	4∗A10 + 2∗A12 + 2∗A1 + 2∗A38	16.95	0	61.82	65.2	16.95	17.9	[83]
$C_{10}H_{11}ClN_2O_4$ (ethyl (2-chloromethyl-2,3-dihydro-5*H*-oxazolo[3,2a]-pyrimidin-5-one)-6-carboxylate)	379.7	2∗A14 + 3∗A15 + 2∗A2 + A1 + A16 + A112 + A114 + A38 + A22∗E22 + A18∗B18 + 2∗A19 + A119 + A118	5.38	14.27					[234]
	413.4		10.77	26.1	40.24	72.2	26.08	29.9	
$C_{10}H_{11}NO_3$ (*N*-[4-(acetyloxy)phenyl] acetamide)	427.5	4∗A10 + 2∗A1 + 2∗A12 + A38 + A60	30.97	0	72.44	59.0	30.97	25.2	[69]
$C_{10}H_{11}N_3O_3S$ (4-amino-*N*-(5-methyl-3-isoxazolyl)benzene sulfonamide (sulfamethoxazole))	440.0	4∗A10 + 2∗A12 + A14 + A15 + A1 + A45 + A95 + A118 + A112 + A18 + 2∗A19	35.26	0	80.14	76.2	35.26	33.5	[182]
$C_{10}H_{11}N_5O_3$ (3,9-dihydro-3-[(2-hydroxyethoxy)methyl]-9-oxo-5*H*-imidazol[1,2a]pyrine)	520.6	3∗A14 + 3∗A15 + 3∗A2 + A32 + 3∗A18∗B18 + 3∗A19 + A125 + A121 + 2∗A118 + A119 + A30∗E30	43.33	0	83.23	73.9	43.33	38.5	[31]
$C_{10}H_{12}N_2O_4$ (2,3′-didehydro-3′-deoxythymidine (stavudine))	443.2	2∗A14 + 5∗A15 + A124 + A125 + A19 + A18∗B18 + 2∗A18 + 2∗A16 + A112 + A2 + A1 + A30∗F30	26.91	0	60.7	66.5	26.9	29.5	[203]
$C_{10}H_{12}N_2O_4S$ ((4-nitrophenyl)-2-(methylthio)ethyl carbamate)	349.4	A1 + 2∗A2 + A84 + A69 + 4∗A10 + 2∗A12 + A50	31.27	0	89.50	73.9	31.27	25.8	[114]
$C_{10}H_{12}O$ (4-methoxy-α-methylstyrene)	309.2	2∗A1 + 4∗A10 + 2∗A12 + A5 + A7 + A32	19.07	0	61.68	61.1	19.07	18.9	[34]

$C_{10}H_{14}O_2$ ((1*S*)-(+)-camphorquinone)	473.2	2∗A14 + A15 + 3∗A1 + 2∗A17 + A16 + 2∗A114 (fusion enthalpy seems low, compound may have an unmeasured phase transition at a lower temperature)	6.07	0	12.83	36.6	6.07	17.32	[237][e]
$C_{10}H_{14}N_2O_4$ (2,2-dinitroadamantane)	362.2	3∗A14 + A15 + 4∗A16 + A17 + 2∗A50	16.76	46.27					[122]
	491.2		5.06	10.30	56.57	45.9	21.82	22.6	
$C_{10}H_{14}N_4O_4$ (7-(2,3-dihydroxypropyl)-3,7-dihydro-1,3-dimethyl-1*H*-purine-2,6-dione (dyphylline))	435.7	2∗A14 + 3∗A15 + 2∗A1 + 2∗A2 + 2∗A125 + A119 + A118 + 2∗A19 + A18∗B18 + 2∗A30∗F30 + A3∗B3	39.3	0	90.2	72.1	39.3	31.4	[232]
$C_{10}H_{14}O_2$ (2-*tert*-butyl-1,4-dihydroxybenzene)	350.9	3∗A1 + A4 + 2∗A31 + 3∗A10 + A11 + 2∗A12	27.74	0	79.05	56.2	27.74	19.7	[50]
$C_{10}H_{14}O_2$ (4-*tert*-butyl-1,2-dihydroxybenzene)	330.4	3∗A1 + A4 + 2∗A31 + 3∗A10 + A11 + 2∗A12	15.1	0	45.70	56.2	15.1	18.6	[179]
$C_{10}H_{15}NO$ ((+) *threo*-2-(methylamino)-1-phenyl-1-propanol (pseudoephedrine))	392.4	5∗A10 + 2∗A1 + 2∗A3∗B3 + A12 + A44 + A30∗B30	31.95	0	81.42	55.3	31.95	21.7	[71]
$C_{10}H_{15}NO$ ((±) *threo*-2-(methylamino)-1-phenyl-1-propanol (pseudoephedrine))	391.1	5∗A10 + 2∗A1 + 2∗A3∗B3 + A12 + A44 + A30∗B30	34.10	0	87.19	55.3	34.10	21.7	[71]
$C_{10}H_{15}NO$ ((−) 2-(methylamino)-1-phenyl-1-propanol (ephedrine))	312.9	5∗A10 + 2∗A1 + 2∗A3∗B3 + A12 + A44 + A30∗B30	17.33	0	55.39	55.3	17.33	17.3	[71]
$C_{10}H_{15}NO$ ((±) 2-(methylamino)-1-phenyl-1-propanol (ephedrine))	350.7	5∗A10 + 2∗A1 + 2∗A3∗B3 + A12 + A44 + A30∗B30	29.09	0	82.95	55.3	29.09	19.4	[71]
$C_{10}H_{15}NO_2$ (1-nitroadamantane)	435.2	3∗A14 + A15 + 3∗A16 + A17 + A50 (entropy seems low, compound may have lower temperature phase transitions)	4.18	0	9.60	42.9	4.18	18.7	[122]
$C_{10}H_{15}NO_2$ (2-nitroadamantane)	452.2	3∗A14 + A15 + 5∗A16 + A50 (entropy seems low, compound may have lower temperature phase transitions)	4.23	0	9.23	48.1	4.18	21.8	[122]
$C_{10}H_{16}$ (adamantane)	208.6	3∗A14 + A15 + 2∗A16	3.38	16.20					[125,126]
	543.2		13.80	25.41	41.61	45.1	17.18	24.4	
$C_{10}H_{16}N_2$ ((1,1-dimethylpropyl)-ethylpropanedinitrile)	307.5	4∗A1 + 2∗A2 + A4∗A4 + B4 + 2∗A56	19.25	0	62.60	62.26	19.25	19.1	[76]
$C_{10}H_{16}N_2$ (*meso*-2,3-diethyl-2,3-dimethylsuccinonitrile)	370.2	4∗A1 + 2∗A4∗B4 + 2∗A2 + 2∗A56	26.78	0	72.34	74.06	26.78	27.4	[168]
$C_{10}H_{16}N_6S$ (*N*-cyano-*N*′-methyl-*N*″-[2-[(5-methyl-1*H*-imidazol-4-yl)-thio]ethyl]quanidine (cimetidine))	413.8	2∗A1 + A14 + 2∗A15 + 2∗A19 + A18∗B18 + A118 + A121 + 3∗A2 + A84 + 2∗A44 + A56 + A42 + A7	41.0	0	99.08	69.03	41.00	28.6	[90]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{10}H_{18}O_2$ ((−) 5-hydroxy-α,α,4-trimethyl-3-cyclohexene-1-methanol (*trans*-sobrerol))	423.6	3∗A1 + A14 + 3∗A15 + A4∗B4 + 2∗A30∗B30 + 2∗A16 + A18 + A19	34.69	0	81.89	66.3	34.69	28.1	[71]
$C_{10}H_{18}O_2$ ((±) 5-hydroxy-α,α,4-trimethyl-3-cyclohexene-1-methanol (*trans*-sobrerol))	404.9	3∗A1 + A14 + 3∗A15 + A4∗B4 + 2∗A30∗B30 + 2∗A16 + A18 + A19	34.39	0	84.93	66.3	34.39	26.9	[71]
$C_{10}H_{18}O_2$ ((−) 5-hydroxy-α,α,4-trimethyl-3-cyclohexene-1-methanol (*cis*-sobrerol))	382.9	3∗A1 + A14 + 3∗A15 + A4∗B4 + 2∗A30∗B30 + 2∗A16 + A18 + A19	23.18	0	60.54	66.3	23.18	25.4	[71]
$C_{10}H_{18}O_2$ ((±) 5-hydroxy-α,α,4-trimethyl-3-cyclohexene-1-methanol (*cis*-sobrerol))	378.9	3∗A1 + A14 + 3∗A15 + A4∗B4 + 2∗A30∗B30 + 2∗A16 + A18 + A19	25.86	0	68.25	66.3	25.86	25.1	[71]
$C_{10}H_{18}O_3$ (1-*tert*-butyl-4-methyl-2,6,7-trioxabicyclo[2.2.2]octane)	375.2	2∗A14 + 2∗A15 + 3∗A112 + 4∗A1 + A4 + 2∗A17	16.4	0	43.71	44.2	16.4	16.6	[86]
$C_{10}H_{18}O_6S$ (diethyl-3,3′-sulfonyldipropionate)	359.7	2∗A1 + 6∗A2 + 2∗A38 + A88	38.0	0	105.6	93.5	38.0	33.6	[62]
$C_{11}H_7N_3$ (2,2-dicyano-3-phenylpropionitrile)	411.2	5∗A10 + A11 + A2 + A4∗B4 + 3∗A56	29.29	0	71.23	64.6	29.29	26.6	[74]
$C_{11}H_8F_3N_3O_7$ (2,3-dihydro-6-nitro-3-[2-(nitrooxy)ethyl]-7-(trifluoromethyl)-4*H*-1,3-benzoxazin-4-one)	384.7	A14 + 3∗A15 + 2∗A2 + A125 + A112 + 2∗A19 + A55 + 2∗A10 + A11 + A12 + A50 + 3∗A25 + A4∗B4	28.9	0	75.13	70.3	28.9	27.1	[165]
$C_{11}H_9N$ (4-phenylpyridine)	346.9	9∗A10 + 2∗A12 + A41	19.95	0	57.51	62.5	19.95	21.7	[94]
$C_{11}H_{10}O_2$ (pentacyclo[5.4.0.0.[2,6].0.[3,10].0[5,9]]undecane-8,11-dione)	309.8	5∗A14-4∗A15 + 8∗A16 + 2∗A114	0.32	1.03					[36]
	345.3		9.61	27.83					
	516.8		5.23	10.12	38.98	31.8	15.16	16.4	
$C_{11}H_{12}BrN_5O_3$ (2-bromo-6-methyl-3,9-dihydro-3-[(2-hydroxyethoxy)-methyl]-9-oxo-5*H*-imidazol-[1,2a]pyrine)	474.3	A1 + 3∗A14 + 3∗A15 + 3∗A2 + A32 + A18∗B18 + 5∗A19 + A125 + A121 + 2∗A118 + A119 + A21 + A30∗F30	50.44	0	106.3	92.3	50.44	43.8	[31]
$C_{11}H_{12}I_3NO_2$ ((−) 3-[3-(amino-2,4,6-triiodophenyl]-2-ethylpropanoic acid (iopanoic acid))	438.8	A1 + 2∗A2 + A3 + A10 + 4∗A12 + A11 + 3∗A29 + A45 + A36∗E36	25.98	0	59.21	99.5	25.98	43.7	[71]
$C_{11}H_{12}I_3NO_2$ ((±) 3-[3-(amino-2,4,6-triiodophenyl]-2-ethylpropanoic acid (iopanoic acid))	427.0	A1 + 2∗A2 + A3 + A10 + 4∗A12 + A11 + 3∗A29 + A45 + A36∗E36	27.70	0	64.87	99.5	27.70	42.5	[71]

$C_{11}H_{12}N_2O_5$ (2,3-dihydro-6-methyl-3-[2-(nitrooxy)ethyl]-4*H*-1,3-benzoxazin-4-one)	351.2	A14 + 3∗A15 + 2∗A2 + A125 + A112 + 2∗A19 + A55 + 3∗A10 + A11 + A1	27.1	0	77.16	68.2	27.1	24.0	[165]
$C_{11}H_{12}O_2$ (1-phenyl-4,7-dioxaspiro-[2.4]heptane)	303.1	2∗A14 + A15 + 2∗A112 + A16 + A17 + 5∗A10 + A11	22.6	0	74.56	51.0	22.6	15.5	[88]
$C_{11}H_{13}ClF_3N_3O_4S_3$ (6-chloro-3,4-dihydro-2-methyl-3-([2,2,2-trifluoroethyl]-thio)methyl-2*H*-1,2,4-benzothiadiazine-5-sulfonamide-1,1-dioxide (polythiazide))	493.2	A14 + 3∗A15 + A152 + A121 + 2∗A19 + A16 + 2∗A10 + 2∗A12 + A96 + A22∗F22 + 2∗A2 + A84 + A4∗B4 + 3∗A25 + A1	42.67	0	86.52	75.5	42.67	37.3	[183]
$C_{11}H_{13}N_5O_3$ (6-methyl-3,9-dihydro-3-[(2-hydroxyethoxy)methyl]-9-oxo-5*H*-imidazol[1,2a]pyrine)	465.4	A1 + 3∗A14 + 3∗A15 + 3∗A2 + A32 + 2∗A18∗B18 + 4∗A19 + A125 + A121 + 2∗A118 + A119 + A30∗E30	36.06	0	77.48	82.3	36.06	38.3	[31]
$C_{11}H_{14}N_2O_4$ (3-nitro-3-(*p*-nitrophenyl)-pentane)	?	Melting point temperature not reported	20.29				29.29		[98]
$C_{11}H_{15}N_2O_2$ (2-cyano-2-nitroadamantane)	470.2	3∗A14 + A15 + 4∗A16 + A17 + A50 + A56 (entropy seems low, compound may have lower temperature phase transitions)	4.98	0	10.59	45.9	4.98	21.6	[122]
$C_{11}H_{16}N_2O_2S_2$ (*N*-ethyl-*S*-methyl-*N*′-tosylisothiourea)	390.2	3∗A1 + A2 + 4∗A10 + A11 + A12 + A161	35.80	0	91.75	73.4	35.80	28.6	[23]
$C_{11}H_{16}N_2O_2S_2$ (*N*-methyl-*S*-ethyl-*N*′-tosylisothiourea)	414.2	3∗A1 + A2 + 4∗A10 + A11 + A12 + A161	26.50	0	63.98	73.4	26.50	30.4	[23]
$C_{11}H_{16}N_4O_4$ ((−) 4,4′-(1-methyl-1,2-ethanediyl)bis-2,6-piperazinedione (dexrazoxane))	467.6	A1 + 2∗A14 + 6∗A15 + A3∗B3 + A2 + 2∗A119 + 2∗A129	37.82	0	80.88	68.1	37.82	31.8	[71]
$C_{11}H_{16}N_4O_4$ ((±) 4,4′-(1-methyl-1,2-ethanediyl)bis-2,6-piperazinedione (dexrazoxane))	507.4	A1 + 2∗A14 + 6∗A15 + A3∗B3 + A2 + 2∗A119 + 2∗A129	44.98	0	88.65	68.1	44.98	34.5	[71]
$C_{11}H_{16}O$ (2-*tert*-butyl-6-methylphenol)	302.5	4∗A1 + A4 + A31 + 3∗A10 + 2∗A11 + A12	17.32	0	57.26	51.4	17.32	15.5	[63]
$C_{11}H_{17}NO$ ((−) 2-dimethylamino-1-phenyl-1-propanol (methylephedrine))	361.2	3∗A1 + 2∗A3∗B3 + 5∗A10 + A12 + A30∗B30 + A43	30.56	0	84.61	58.1	30.56	21.0	[71]
$C_{11}H_{17}NO$ ((±) 2-dimethylamino-1-phenyl-1-propanol (methylephedrine))	336.0	3∗A1 + 2∗A3∗B3 + 5∗A10 + A12 + A30∗B30 + A43	26.60	0	72.68	58.1	26.60	19.5	[71]
$C_{11}H_{24}B_{10}O_3$ (1,7-dicarbadodecaborane(12)-1-carboperoxoic acid, 7-(1-methylethyl)-1,1-dimethyl-2-propynyl ester)	368.0	Group values are not available	32.4	0	88.04		32.4		[104]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{12}HF_{25}$ (1*H*-perfluorododecane)	345	11∗A4∗B4 + A3∗B3 + 22∗A26 + 3∗A25	21.0	0	60.9	67.8	21.0	23.4	[195]
$C_{12}H_4Cl_4O_2$ (2,3,7,8-tetrachlorodibenzodioxin)	578.2	A14 + 3∗A15 + 2∗A112 + 4∗A22∗F22 + 4∗A19 + 4∗A10 + 4∗A12	38.90	0	67.20	62.10	38.90	35.9	[45]
$C_{12}H_6Cl_2O_2$ (2,3-dichlorodibenzodioxin)	431.6	A14 + 3∗A15 + 2∗A112 + 2∗A22∗D22 + 4∗A19 + 6∗A10 + 2∗A12	27.1	0	62.79	59.5	27.1	25.7	[163]
$C_{12}H_{10}O$ (4-hydroxybiphenyl)	443.1	9∗A10 + A31 + 3∗A12	31.59	0	71.29	64.6	31.59	28.6	[97]
$C_{12}H_{10}O_2$ (2,2′-dihydroxybiphenyl)	386.7	8∗A10 + 2∗A31 + 4∗A12	25.36	0	65.58	69.8	25.36	27.0	[97]
$C_{12}H_{10}O_2$ (4,4′-dihydroxybiphenyl)	560.7	8∗A10 + 2∗A31 + 4∗A12	43.05	0	76.78	69.8	43.05	39.1	[97]
$C_{12}H_{11}N_3O_2S$ (5-nitro-2-thiophene-carboxaldehyde-4-methylphenyl-hydrazone)									
Red greenish plates	425	A14 + 2∗A15 + A1 + 4∗A10 + A11 + A12 + A50 + 2∗A18 + 2∗A19 + A131 + A6∗B6 + A44 + A42	5.23	0	12.3	60.6	5.2	25.8	[218]
Red orange prisms	429.2		15.15	0	35.3	60.6	15.2	26.0	
Black needles	430.2		25.3	0	58.9	60.6	25.3	26.0	
$C_{12}H_{12}N_2O_3$ (1-ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid (nalidixic acid))	501.9	A14 + 3∗A15 + 3∗A19 + A18∗B18 + A119 + A114 + 2∗A10 + A11 + 2∗A1 + A41 + A36∗E36 + A2	35.92	0	71.6	72.4	35.9	36.3	[198]
$C_{12}H_{14}O_3$ (4-methyl-1-phenyl-2,6,7-trioxabicyclo[2.2.2]octane)	410.2	2∗A14 + 2∗A15 + 3∗A112 + A1 + 2∗A17 + 5∗A10 + A11	20.9	0	50.95	53.6	20.9	22.0	[86]
$C_{12}H_{16}N_2O_4$ (pentyl-*N*-(4-nitrophenyl) carbamate)	363.8	A1 + 4∗A2 + A69 + 4∗A10 + 2∗A12 + A50	25.98	0	71.42	88.9	25.98	32.3	[114]
$C_{12}H_{17}NO_2$ (2,6-diisopropylnitrobenzene)	301.2	4∗A1 + 2∗A3 + 3∗A10 + A12 + 2∗A11 + A50	12.51	0	41.53	50.8	12.51	15.3	[230]
$C_{12}H_{17}N_3O_3$ (1-pentyl-3-(4-nitrophenyl) urea)	404.2	A1 + 4∗A2 + A66 + 4∗A10 + 2∗A12 + A50	19.85	0	49.1	79.8	19.85	32.3	[114]
$C_{12}H_{18}N_2O_2S_2$ (*N*-isopropyl-*S*-methyl-*N*′-tosylisothiourea)	392.2	4∗A1 + A3∗B3 + 4∗A10 + A11 + A12 + A161	32.70	0	83.38	73.56	32.70	29.0	[23]
$C_{12}H_{18}N_2O_2S_2$ (*N*-ethyl-*S*-ethyl-*N*′-tosylisothiourea)	390.2	3∗A1 + 2∗A2 + 4∗A10 + A11 + A12 + A161	30.30	0	77.65	80.0	30.30	31.4	[23]
$C_{12}H_{20}N_2$ (1-cyano-1-piperidinocyclohexane)	339.2	2∗A14 + 6∗A15 + A17 + A56 + A119	25.44	0	75.00	52.8	25.44	17.9	[87]
$C_{12}H_{20}O_2$ (bicyclo[2.2.1]heptan-7-one 2,2-dimethylpropylene ketal)	346.7	3∗A14 + 3∗A15 + 2∗A1 + 2∗A112 + 2∗A16 + 2∗A17	23.9	0	68.94	50.3	23.9	17.4	[88]

$C_{12}H_{22}O_{11}$ (α-lactose)	496.2	2∗A14 + 6∗A15 + 10∗A16 + 2∗A2 + 8∗A30∗F30 + 2∗A112 + A32	75.2	0	151.6	141.5	75.2	70.2	[207]
$C_{12}H_{24}O_{11}$ (α-D-glucopyranosyl-1, 6-sorbitol)	439.0	A14 + 3∗A15 + 5∗A16 + 3∗A2 + A32 + A112 + 9∗A30∗F30 + 4∗A3∗B3	56.4	0	128.5	159.3	56.4	69.9	[162]
$C_{12}H_{24}O_{11}$ (α-D-glucopyranosyl-1, 6-mannitol)	440.8	A14 + 3∗A15 + 5∗A16 + 3∗A2 + A32 + A112 + 9∗A30∗F30 + 4∗A3∗B3	55.0	0	124.8	159.3	55.0	70.2	[162]
$C_{12}H_{26}O$ (2,2,4,4-tetramethyl-3-isopropyl-3-pentanol)	314.0	8∗A1 + 2∗A4 + A4∗B4 + A3 + A30 (compound likely has an unmeasured solid phase transition, not used in generating the statistics)	2.09	0	6.66	50.5	2.09	15.9	[62]
$C_{12}H_{26}O_4$ (4,4′-[1,4-butanediylbis-(oxy)]bis-1-butanol)	306.7	12∗A2∗B2 + 2∗A32 + 2∗A30∗D30	39.37	0	139.2	165.6	39.4	42.7	[109]
$C_{12}H_{30}B_8$ (1,10-dipentyl-1, 10-dicarbadecaborane)	269.7	Group values are not available	14.7	0	54.51		14.7		[127]
$C_{12}H_{36}Si_5$ (tetrakis(trimethylsilyl)silane)	241.2	Compound sublimed, fusion values not reported	11.57	47.97					[108]
$C_{13}H_4N_4O_{10}$ (2,3,5,7-tetranitroxanthone)	514.0	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 4∗A10 + 4∗A12 + 4∗A50	33.56	0	65.29	65.5	33.56	33.7	[13]
$C_{13}H_4N_4O_{10}$ (2,4,5,7-tetranitroxanthone)	593.9	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 4∗A10 + 4∗A12 + 4∗A50	32.20	0	54.20	65.5	32.20	38.9	[13]
$C_{13}H_5N_3O_8$ (1,2,7-trinitroxanthone)	554.9	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 5∗A10 + 3∗A12 + 3∗A50 (decomposes near melting point temperature)	11.89	0	21.43	62.7	11.89	34.8	[13]
$C_{13}H_5N_3O_8$ (2,3,7-trinitroxanthone)	538.9	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 5∗A10 + 3∗A12 + 3∗A50	24.91	0	46.22	62.7	24.91	33.8	[13]
$C_{13}H_5N_3O_8$ (2,4,7-trinitroxanthone)	477.8	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 5∗A10 + 3∗A12 + 3∗A50	31.40	0	65.72	62.7	31.40	30.0	[13]
$C_{13}H_6N_2O_6$ (1,7-dinitroxanthone)	536.4	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 6∗A10 + 2∗A12 + 2∗A50	37.23	0	69.41	59.90	37.23	32.1	[13]
$C_{13}H_6N_2O_6$ (2,5-dinitroxanthone)	491.2	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 6∗A10 + 2∗A12 + 2∗A50	31.37	0	63.86	59.90	31.37	29.4	[13]
$C_{13}H_6N_2O_6$ (2,6-dinitroxanthone)	541.0	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 6∗A10 + 2∗A12 + 2∗A50	26.13	0	48.30	59.90	26.13	32.4	[13]
$C_{13}H_6N_2O_6$ (2,7-dinitroxanthone)	540.0	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 6∗A10 + 2∗A12 + 2∗A50	30.59	0	56.65	59.90	30.59	32.3	[13]
$C_{13}H_7NO_4$ (1-nitroxanthone)	477.7	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 7∗A10 + A12 + A50	28.90	0	60.50	57.1	28.90	27.3	[13]
$C_{13}H_7NO_4$ (2-nitroxanthone)	477.9	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 7∗A10 + A12 + A50	26.75	0	55.97	57.1	26.75	27.3	[13]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{13}H_7NO_4$ (3-nitroxanthone)	448.0	A14 + 3∗A15 + 4∗A19 + A112 + A114 + 7∗A10 + A12 + A50	25.37	0	56.63	57.1	25.37	25.6	[13]
$C_{13}H_8N_2O_2$ (1-phenazinecarboxylic acid)	514.5	7∗A10 + 4∗A12 + 2∗A41 + A12 + A36∗B36	35.44	0	68.9	52.3	35.44	26.9	[29]
$C_{13}H_9F_3N_2O_2$ (2-[3-(trifluoromethyl)-anilino)nicotinic acid)	477.2	3∗A25∗ + A4∗B4 + 7∗A10 + 3∗A12 + A11 + A44 + A41 + A36∗F36	32.73	0	68.6	72.4	32.7	34.5	[204]
$C_{13}H_{10}N_4O$ (1-phenazinecarboxylic acid hydrazide)	505.0	7∗A10 + 5∗A12 + 2∗A41 + A147	27.62	0	54.7	63.4	27.62	32.0	[29]
$C_{13}H_{10}O$ (xanthene)	374.3	A14 + 3∗A15 + 2∗A19 + 8∗A10 + A112 + 2∗A19	15.87	0	42.40	55.7	15.87	20.8	[129]
$C_{13}H_{10}O_3$ (diphenyl carbonate)	355.0	10∗A10 + 2∗A12 + A149	23.43	0	66.00	66.0	23.43	23.4	[93]
$C_{13}H_{10}O_4$ (2,4,4′-trihydroxybenzophenone)	482.6	7∗A10 + 5∗A12 + A35 + 3∗A31	31.3	0	64.86	79.8	31.3	38.5	[136]
$C_{13}H_{10}O_5$ (2,2′,4,4′-tetrahydroxybenzophenone)	472.0	6∗A10 + 6∗A12 + A35 + 4∗A31	28.0	0	59.32	85.2	28.0	40.2	[136]
$C_{13}H_{13}NO$ (2-(4-methoxyphenyl)-5-methylpyridine)	328	7∗A10 + 4∗A12 + A1 + A32 + A41	20.0	0	61.0	55.0	20	18.0	[199]
$C_{13}H_{16}N_2$ (2-phenyl-2-piperidinoacetonitrile)	335.2	A14 + 3∗A15 + A3∗B3 + 5∗A10 + A11 + A56 + A119	19.71	0	58.80	60.5	19.71	20.3	[87]
$C_{13}H_{16}N_2O_6$ (2,3-dihydro-7-(1-methylethoxy)-3-[2-(nitrooxy)ethyl]-4*H*-1,3-benzoxazin-4-one)	344.7	A14 + 3∗A15 + 2∗A2 + A125 + A112 + 2∗A19 + A55 + 3∗A10 + A12 + 2∗A1 + A3∗B3 + A32	32.1	0	93.12	82.8	32.1	28.5	[165]
$C_{13}H_{16}N_2O_7$ (2-methylpropanoic acid 2,3-dihydro-7-(1-methylethoxy)-3-[2-(nitrooxy)ethyl]-4-oxo-2*H*-1,3-benzoxazin-7-yl ester)	345.7	A14 + 3∗A15 + 2∗A2 + A125 + A112 + 2∗A19 + A55 + 3∗A10 + A12 + 2∗A1 + A3∗B3 + A38	26.0	0	75.21	85.8	26.0	29.6	[165]
$C_{13}H_{17}ClN_2O_4$ ((4-nitrophenyl)-6-chlorohexyl carbamate)	360.8	6∗A2 + A69 + 4∗A10 + 2∗A12 + A50 + A22∗C22	30.31	0	84.01	98.8	30.31	35.6	[114]
$C_{13}H_{18}N_2O_2S_2$ (*N*-allyl-*S*-ethyl-*N*′-tosylisothiourea)	335.2	A5 + A6 + 2∗A2 + 2∗A1 + 4∗A10 + A11 + A12 + A161	28.00	0	83.53	85.5	28.00	28.6	[23]
$C_{13}H_{18}N_2O_4$ (hexyl-*N*-(4-nitrophenyl) carbamate)	376.7	A1 + 5∗A2 + A69 + 4∗A10 + 2∗A12 + A50	32.74	0	86.91	93.1	32.74	35.1	[114]
$C_{13}H_{18}O_2$ ((−) α-methyl-4-(isobutyl)phenylacetic acid (ibuprofen))	327.2	3∗A1 + A2 + 4∗A10 + 2∗A11 + A3 + A3∗B3 + A36	17.90	0	54.71	57.5	17.90	18.8	[71]

$C_{13}H_{18}O_2$ ((±) α-methyl-4-(isobutyl)-phenylacetic acid (ibuprofen))	350.9	3∗A1 + A2 + 4∗A10 + 2∗A11 + A3 + A3∗B3 + A36	25.70	0	73.24	57.5	25.70	20.2	[71]
$C_{13}H_{19}NO_4$ (*N*-phenylethyl-5-amino-1, 5-dideoxy-D-glucopyranose)	455.8	A14 + 3∗A15 + 4∗A16 + A119 + 4∗A30∗E30 + 2∗A2 + 5∗A10 + A11	39.9	0	87.54	90.3	39.9	41.1	[25]
$C_{13}H_{19}N_3O_3$ (1-hexyl-3-(4-nitrophenyl) urea)	384.4	A1 + 5∗A2 + A66 + 4∗A10 + 2∗A12 + A50	25.47	0	66.26	86.9	25.47	33.4	[114]
$C_{13}H_{20}N_2O_2S_2$ (*N*-isobutyl-*S*-methyl-*N*′-tosylisothiourea)	363.2	4∗A1 + A2 + A3 + 4∗A10 + A11 + A12 + A161	29.40	0	80.95	74.6	29.40	27.1	[23]
$C_{13}H_{20}N_2O_2S_2$ (*N*-*tert*-butyl-*S*-methyl-*N*′-tosylisothiourea)	394.2	5∗A1 + A4∗B4 + 4∗A10 + A11 + A12 + A161	30.40	0	77.12	78.5	30.40	30.9	[23]
$C_{13}H_{20}N_2O_2S_2$ (*N*-isopropyl-*S*-ethyl-*N*′-tosylisothiourea)	392.2	A2 + 4∗A1 + A3∗B3 + 4∗A10 + A11 + A12 + A161	29.10	0	74.20	81.1	29.10	31.8	[23]
$C_{13}H_{22}$ (1,3,5-trimethyladamantane)	234.4		8.19	34.94					
	255.6	3∗A14 + A15 + A16 + 3∗A17 + 3∗A1	2.06	8.06	43.0	38.2	10.25	9.76	[137]
$C_{13}H_{28}O_2$ (1,13-tridecanediol)	343.0	2∗A30∗B30 + 13∗A2∗B2	28.90	86.88					[15]
	351.0		17.80	50.71	137.6	156.2	46.70	54.8	
$C_{14}H_9Cl$ (1-chloroanthracene)	355.2	9∗A10 + 5∗A12 + A22	14.14	0	39.81	39.9	14.14	14.2	[110]
$C_{14}H_9Cl$ (9-chloroanthracene)	379.2	9∗A10 + 5∗A12 + A22	18.66	0	49.21	39.9	18.66	15.1	[110]
$C_{14}H_9N_3O_2S$ (5-methyl-[(2-nitrophenyl)amino]-3-thiophene carbonitrile)									
Yellow prism	383.0	A14 + 2∗A15 + 3∗A19 + A18 + A1 + A131 + A56 + A50 + 4∗A10 + 2∗A12 + A44	27.2	0	71.02	67.5	27.2	25.9	[113]
Orange needle	388.0		25.1	0	64.69	67.5	25.1	26.2	
Orange prism	385.9		25.5	0	66.08	67.5	25.5	26.0	
Red prism	379.4		26.0	0	68.53	67.5	26.0	25.6	
$C_{14}H_{10}F_4$ (1,1,2,2-tetrafluoro-1, 2-diphenylethane)	399.2	10∗A10 + 2∗A11 + 4∗A26 + 2∗A4∗B4	28.83	0	72.22	61.7	28.83	24.6	[95]
$C_{14}H_{10}N_2O_2$ (*N*-anilinophthalimide)	401.0	A14 + 2∗A15 + 9∗A10 + A12 + A128 + 2∗A19 + A44	1.62	4.04					[156]
	457.0		26.9	58.86	62.90	66.8	28.52	30.5	
$C_{14}H_{10}O_4$ (diphenyl oxalate)	403.0	10∗A10 + 2∗A12 + A38	31.38	0	77.87	66.7	31.38	26.9	[93]
$C_{14}H_{10}O_4$ (benzoyl peroxide)	378.0	Group values not available (large uncertainty in reported value, compound may undergo some decomposition upon melting)	22.59	0	59.74		22.59		[140]
$C_{14}H_{11}F_3$ (1,1,2-trifluoro-1, 2-diphenylethane)	364.2	10∗A10 + 2∗A11 + 2∗A26 + A27 + A4∗B4 + A3∗B3	28.37	0	77.90	61.1	28.37	22.2	[95]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{14}H_{11}IO_3S$ (4-(2-propenyloxy)-phenyl-5-iodo-2-thiophene carboxylate)	383.2	A14 + 2∗A15 + 4∗A10 + 2∗A12 + A5 + A6 + 2∗A18 + 2∗A19 + A131 + A29 + A32 + A38 + A2 (not used in generating the statistics; experimental values in this article appear significantly out of line with both related molecules and estimations)	83.68	0	218.4	92.0	83.68	35.3	[230]
$C_{14}H_{12}ClN$ (4-chlorobenzylidene-4′-methylaniline)	400.4	8∗A10 + 3∗A12 + A11 + A6∗B6 + A42 + A22∗B22 + A1	25.58	0	63.9	63.1	25.58	25.3	[219]
$C_{14}H_{12}F_2$ (1,1-difluoro-1,2-diphenylethane)	339.2	10∗A10 + 2∗A11 + A2 + A4∗B4 + 2∗A26	24.35	0	71.79	65.3	24.35	22.2	[95]
$C_{14}H_{12}O_4$ (2,4-dihydroxy-4′-methoxybenzophenone)	436.8	7∗A10 + 5∗A12 + A35 + 2∗A31 + A1 + A32	35.6	0	81.50	81.8	35.6	35.7	[136]
$C_{14}H_{12}O_4$ (2,2′-dihydroxy-4-methoxybenzophenone)	343.0	7∗A10 + 5∗A12 + A35 + 2∗A31 + A1 + A32	22.0	0	64.14	81.8	22.0	28.1	[136]
$C_{14}H_{14}$ (5,6-dimethylacenaphthene)	443.2	4∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + 2∗A11	21.76	0	49.10	42.0	21.76	18.6	[55]
$C_{14}H_{14}$ (3,8-dimethylacenaphthene)	341.7	4∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + 2∗A11	17.99	0	52.65	42.0	17.99	14.4	[55]
$C_{14}H_{14}$ (4,7-dimethylacenaphthene)	314.2	4∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + 2∗A11	15.06	0	47.93	42.0	15.06	13.2	[55]
$C_{14}H_{14}$ (3,4-dimethylacenaphthene)	357.2	4∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + 2∗A11	17.57	0	49.19	42.0	17.57	15.0	[55]
$C_{14}H_{14}$ (1,3-dimethylacenaphthene)	283.2	5∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + A11 + A16	12.55	0	44.32	44.3	12.55	12.5	[55]
$C_{14}H_{14}$ (1,5-dimethylacenaphthene)	316.7	5∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + A11 + A16	22.18	0	70.03	44.3	22.18	14.0	[55]
$C_{14}H_{14}$ (1,8-dimethylacenaphthene)	289.2	5∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + A11 + A16	14.23	0	49.20	44.3	14.23	12.8	[55]
$C_{14}H_{14}$ (1,7-dimethylacenaphthene)	288.2	5∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + A11 + A16	14.23	0	49.38	44.3	14.23	12.8	[55]
$C_{14}H_{14}$ (1,4-dimethylacenaphthene)	279.7	5∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + A11 + A16	17.57	0	62.82	44.3	17.57	12.4	[55]
$C_{14}H_{14}$ (1,2-*cis*-dimethylacenaphthene)	325.2	6∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + 2∗A16	22.59	0	69.46	46.6	22.59	15.25	[55]
$C_{14}H_{14}$ (1,2-*trans*-dimethylacenaphthene)	350.2	6∗A10 + A14 + 2∗A15 + 3∗A19 + A12 + 2∗A1 + 2∗A16	18.83	0	53.77	46.6	18.83	16.3	[55]
$C_{14}H_{14}O$ (1,1-diphenylethanol)	357.9	10∗A10 + 2∗A11 + A1 + A30 + A4∗B4	26.49	0	74.02	51.13	26.49	18.3	[72]

$C_{14}H_{15}NO$ (2-(4-ethoxyphenyl)-5-methylpyridine)	364	7∗A10 + 4∗A12 + A1 + A32 + A41 + A2	21.0	0	57.7	62.1	21.0	23.9	[199]
$C_{14}H_{18}Fe$ (1,1′-diethylferrocene)	236.9	Group values not available	21.03	0	88.77		21.03		[100]
$C_{14}H_{18}N_4O_3$ (5-[(3,4,5-trimethoxyphenyl)methyl]-2,4-pyrimidinediamine (trimethoprim))	474.0	3∗A1 + 3∗A32 + 3∗A10 + 5∗A12 + A11 + A2 + 2∗A41 + 2∗A45	53.65	0	113.2	104.1	53.65	49.4	[182]
$C_{14}H_{18}O_3$ ((E)(+) 4,4-dimethyl-1-(3,4-methylenedioxyphenyl)-1-penten-3-ol (stiripentol))	348.2	A14 + 2∗A15 + 3∗A10 + A12 + 2∗A19 + 2∗A112 + A30∗C30 + 3∗A1 + A4 + A3∗B3 + 2∗A6	29.0	0	83.29	68,6	29.0	23.9	[120]
$C_{14}H_{18}O_2$ (6,6-dimethyl-1-phenyl-4,8-dioxaspiro[2.5]octane)	351.2	2∗A14 + 2∗A15 + 2∗A1 + 2∗A112 + 5∗A10 + A11 + 2∗A17 + A16	27.2	0	77.45	55.3	27.2	19.4	[88]
$C_{14}H_{19}N_5O_3$ (6-*tert*-butyl-3,9-dihydro-3-[(2-hydroxyethoxy)methyl]-9-oxo-5*H*-imidazol[1,2a]pyrine)	478.5	3∗A1 + A4 + 3∗A14 + 3∗A15 + 3∗A2 + A32 + 2∗A18∗B18 + 4∗A19 + A125 + A121 + 2∗A118 + A119 + A30∗E30	37.95	0	73.31	82.7	37.95	39.6	[31]
$C_{14}H_{20}N_2O$ (*N*-(2,6-dimethylphenyl)-2-piperidinecarboxamide)	403.2	2∗A1 + 3∗A10 + 2∗A11 + A12 + A14 + 3∗A15 + A61 + A16 + A119	24.19	0	60.00	69.1	24.19	27.9	[139]
$C_{14}H_{20}N_2O_2$ ((−) 1-(1*H*-indol-4-yloxy)-3-(isopropylamino)-2-propanol (pindolol))	365.7	3∗A10 + A12 + A14 + 2∗A15 + A18 + A18∗B18 + 2∗A19 + A121 + 2∗A1 + 2∗A2 + 2∗A3∗B3 + A30∗D30 + A32 + A44	25.69	0	70.25	79.8	25.69	29.2	[71]
$C_{14}H_{20}N_2O_2$ ((±) 1-(1*H*-indol-4-yloxy)-3-(isopropylamino)-2-propanol (pindolol))	442.9	3∗A10 + A12 + A14 + 2∗A15 + A18 + A18∗B18 + 2∗A19 + A121 + 2∗A1 + 2∗A2 + 2∗A3∗B3 + A30∗D30 + A32 + A44	57.90	0	130.7	79.8	57.90	35.4	[71]
$C_{14}H_{22}N_2O_3$ ((+) 4-[2′-hydroxy-3′-(isopropylamino)propoxy]-phenylacetamide (atenolol))	420.3	2∗A1 + 3∗A2 + 2∗A3∗B3 + 4∗A10 + A11 + A12 + A44 + A30∗D30 + A32 + A61	36.77	0	87.49	98.9	36.77	41.6	[71]
$C_{14}H_{22}N_2O_3$ ((±) 4-[2′-hydroxy-3′-(isopropylamino)propoxy]-phenylacetamide (atenolol))	423.4	2∗A1 + 3∗A2 + 2∗A3∗B3 + 4∗A10 + A11 + A12 + A44 + A30∗D30 + A32 + A61	35.66	0	84.22	98.9	35.66	41.9	[71]
$C_{14}H_{22}O_2$ (2,5-di-*tert*-butyl-1,4-dihydroxybenzene)	496.5	6∗A1 + 2∗A4 + 2∗A31 + 2∗A10 + 2∗A11 + 2∗A12	43.85	0	88.3	57.2	43.85	28.4	[50]
$C_{14}H_{22}O_2$ (3,5-di-*tert*-butyl-1,2-dihydroxybenzene)	372.8	6∗A1 + 2∗A4 + 2∗A31 + 2∗A10 + 2∗A11 + 2∗A12	24.1	0	64.65	57.2	24.1	21.3	[179]
$C_{14}H_{26}O_6S$ (dibutyl-3,3′-sulfonyldipropionate)	344.0	2∗A1 + 10∗A2 + 2∗A38 + A88	31.4	0	91.28	121.9	31.4	41.9	[62]
$C_{14}H_{30}O_2$ (1,14-tetradecanediol)	360.4	2∗A30∗B30 + 14∗A2∗B2	61.90	0	171.8	165.6	61.90	59.7	[15]
$C_{14}H_{30}O_4S_2$ (2-deoxy-D-glucose dibutyl dithioacetal)	409.5	2∗A1 + 8∗A2 + 4∗A3∗B3 + 2∗A84 + 4∗A30∗F30	60.3	0	147.3	145.9	60.3	59.8	[238]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{14}H_{30}O_5S_2$ (D-glucose dibutyl dithioacetal)	399.0	2∗A1 + 7∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	50.2	0	125.8	151.3	50.2	60.3	[238]
$C_{14}H_{30}O_5S_2$ (L-rhamnose dibutyl dithioacetal)	389.9	2∗A1 + 7∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30 (authors report that there are several transitions prior to melting)	37.9	0	97.20	151.3	37.9	59.0	[238]
$C_{14}H_{30}O_5S_2$ (L-arabinose dibutyl dithioacetal)	380.4	2∗A1 + 7∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	41.5	0	109.1	151.3	41.5	57.5	[238]
$C_{14}H_{30}O_5S_2$ (D-galactose dibutyl dithioacetal)	399.2	2∗A1 + 7∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	46.4	0	116.2	151.3	46.4	60.4	[238]
$C_{15}H_9N$ (9-cyanoanthracene)	445.2	9∗A10 + 5∗A12 + A56	25.19	0	56.58	46.8	25.19	20.8	[110]
$C_{15}H_{10}Cl_2N_2O_2$ (1-[(2,4-dichlorophenyl)methyl]-1*H*-indazole-3-carboxylic acid)	480.2	A14 + 2∗A15 + 3∗A19 + A118 + A119 + 7∗A10 + 2∗A12 + A11 + A2 + A36∗C36 + 2∗A22∗C22	45.92	0	95.63	82.0	45.92	39.4	[226]
$C_{15}H_{10}O$ (9-anthraldehyde)	377.2	9∗A10 + 5∗A12 + A34	17.61	0	46.69	50.6	17.61	19.1	[110]
$C_{15}H_{10}O$ (5,7-dihydro-6*H*-dibenzo-[a,c]cyclohepten-6-one)	350.3	A14 + 4∗A15 + 4∗A19 + A18 + A18∗B18 + A114 + 8∗A10	18.16	0	51.84	52.1	18.16	18.3	[14]
$C_{15}H_{11}ClN_2O$ (7-chloro-1,3-dihydro-5-phenyl-2*H*-1,4-benzodiazepin-2-one (nordazepam))									
Form I	494.5	A14 + 4∗A15 + A22∗C22 + 8∗A10 + 2∗A12 + A124 + A118 + 3∗A19 (melting point temperature and predictive formula given incorrectly in earlier paper)	24.45	0	49.44	74.9	24.45	37.04	[177]
Form II	489.9		34.00	0	69.40	74.9	34.00	36.69	
Form III	489.2		27.40	0	56.01	74.9	27.40	36.64	
Form IV	487.4		33.62	0	68.98	74.9	33.62	36.66	
$C_{15}H_{11}NO_3S$ (4-(2-propenyloxy)-phenyl-5-cyano-2-thiophene carboxylate)	361.5	A14 + 2∗A15 + 4∗A10 + 2∗A12 + A5 + A6 + 2∗A18 + 2∗A19 + A131 + A56 + A32 + A38 + A2 (not used in generating the statistics; experimental values in this article appear significantly out of line with both related molecules and estimations)	103.8	0	287.0	90.31	103.8	32.6	[230]
$C_{15}H_{12}N_2O_2$ (*N*-(*N*′-methylanilino)phthalamide)	374.0	A14 + 2∗A15 + 9∗A10 + A12 + A128 + 2∗A19 + A1 + A43	3.60	9.63					[156]
	399.0		21.7	54.39	64.02	67.5	25.3	26.9	

$C_{15}H_{12}O$ (dibenzosuberone)	305.5	A14 + 4∗A15 + 8∗A10 + A114 + 4∗A19	17.15	0	56.14	56.8	17.15	17.35	[14]
$C_{15}H_{13}N_3O_4S$ (2*H*-1,2-benzothiazine-3-carboxyamide-4-hydroxy-2-methyl-*N*-2-pyridinyl-1,1-dioxide (piroxicam))	474.5	8∗A10 + A14 + 3∗A15 + 4∗A19 + A137 + A60 + A30∗C30 + A41 + A12	35.00	0	73.77	75.49	35.00	35.82	[61]
$C_{15}H_{14}ClN$ (4-chlorobenzylidene-4′-ethylaniline)	358.4	8∗A10 + 3∗A12 + A11 + A6∗B6 + A42 + A22∗B22 + A1 + A2	17.21	0	48.02	70.2	17.21	25.2	[219]
$C_{15}H_{14}O_2$ (2,2-diphenyl-1,3-dioxalane)	328.1	A14 + 2∗A15 + 2∗A112 + 10∗A10 + 2∗A11 + A17	15.9	0	48.46	63.4	15.9	20.8	[88]
$C_{15}H_{14}O_2$ (4,4′-dihydroxy-α-methylstilbene)	465.2	8∗A10 + 4∗A12 + A6 + A7 + A1 + 2∗A31 (DSC thermogram showed an unquantified transition between 373 and 393 K)	20.82	0	44.75	82.0	20.83	38.1	[184]
$C_{15}H_{14}O_4$ (2-hydroxy-4, 4′-dimethoxybenzophenone)	390.4	7∗A10 + 5∗A12 + A35 + A31 + 2∗A1 + 2∗A32	37.6	0	96.31	83.8	37.6	32.7	[136]
$C_{15}H_{14}O_4S$ (4-(2-propenyloxy)-phenyl-5-methoxy-2-thiophene carboxylate)	336.9	A14 + 2∗A15 + 4∗A10 + 2∗A12 + A5 + A6 + 2∗A18 + 2∗A19 + A131 + A1 + 2∗A32 + A38 + A2 (not used in generating the statistics; experimental values in this article appear significantly out of line with both related molecules and estimations)	66.94	0	198.7	94.9	66.94	32.0	[230]
$C_{15}H_{14}O_5$ (2,2′-dihydroxy-4, 4′-dimethoxybenzophenone)	412.3	6∗A10 + 6∗A12 + A35 + 2∗A31 + 2∗A1 + 2∗A32	33.2	0	80.52	89.2	33.2	36.8	[136]
$C_{15}H_{15}NO_2$ (2-[(2,3-dimethylphenyl)-amino]benzoic acid)	503.6	7∗A10 + 2∗A11 + 3∗A12 + 2∗A1 + A36∗B36 + A44	38.2	0	75.9	56.2	38.2	28.3	[201]
$C_{15}H_{16}O_2$ (dimethoxydiphenylmethane)	380.0	10∗A10 + 2∗A11 + 2∗A1 + A4∗B4 + 2∗A32	27.8	0	73.16	76.5	27.8	29.1	[88]
$C_{15}H_{22}N_2O$ (*N*-(2,6-dimethylphenyl)-1-methyl-2-piperidinecarboxamide)	426.2	3∗A1 + 3∗A10 + 2∗A11 + A12 + A14 + 3∗A15 + A60 + A16 + A119	17.77	0	41.69	72.0	17.77	30.7	[139]
$C_{15}H_{22}N_2O_4$ (octyl-*N*-(4-nitrophenyl) carbamate)	383.6	A1 + 7∗A2 + A69 + 4∗A10 + 2∗A12 + A50	38.85	0	101.2	107	38.85	41.2	[114]
$C_{15}H_{22}N_2O_5$ ((4-nitrophenyl)-8-hydroxyoctyl carbamate)	386.9	8∗A2 + A69 + 4∗A10 + 2∗A12 + A50 + A30∗C30	44.07	0	113.9	113.3	44.07	43.8	[114]
$C_{15}H_{23}NO_2$ ((+) 1-(*o*-allylphenoxy)-3-(isopropylamino)-2-propanol (alprenolol))	298.5	2∗A1 + 4∗A10 + A11 + A12 + 3∗A2 + 2∗A3∗B3 + A5 + A6 + A32 + A44 + A30∗C30	23.78	0	79.66	87.8	23.78	26.2	[71]
$C_{15}H_{23}NO_2$ ((±) 1-(*o*-allylphenoxy)-3-(isopropylamino)-2-propanol (alprenolol))	331.2	2∗A1 + 4∗A10 + A11 + A12 + 3∗A2 + 2∗A3∗B3 + A5 + A6 + A32 + A44 + A30∗C30	35.61	0	107.5	87.8	35.61	29.1	[71]
$C_{15}H_{23}N_3O_4S$ ((−) *N*-1-(ethylpyrrolidin-2-ylmethyl)-2-methoxy-5-sulfamoylbenzamide (sulpiride))	459.5	A14 + 2∗A15 + 2∗A1 + 2∗A2 + 3∗A10 + 3∗A12 + A96 + A16 + A119 + A32 + A60	42.01	0	91.43	90.5	42.01	41.6	[71]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{15}H_{23}N_3O_4S$ ((±) *N*-1-(ethylpyrrolidin-2-ylmethyl)-2-methoxy-5-sulfamoylbenzamide (sulpiride))	451.0	A14 + 2∗A15 + 2∗A1 + 2∗A2 + 3∗A10 + 3∗A12 + A96 + A16 + A119 + A32 + A60	46.15	0	102.3	90.5	46.15	40.8	[71]
$C_{15}H_{24}O$ (2,6-di-*tert*-butyl-4-methylphenol)	341.7	7∗A1 + 2∗A10 + 3∗A11 + A12 + 2∗A4 + A31	19.85	0	58.09	52.4	19.85	17.9	[63]
$C_{15}H_{32}O_2$ (1,15-pentadecanediol)	349.4	2∗A30∗B30 + 15∗A2∗B2	35.10	100.5					[15]
	361.4		23.60	65.3	165.8	174.9	58.70	63.21	
$C_{15}H_{32}O_4$ (5,5′-[1,5-pentanediylbis(oxy)]*bis*-1-pentanol)	302.7	15∗A2∗B2 + 2∗A30∗E30 + 2∗A32	35.66	0	117.8	174.8	35.66	63.2	[109]
$C_{16}H_{13}ClN_2O_2$ (7-chloro-1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-2*H*-1,4-benzodiazepin-2-one (temazepam))	432.6	A14 + 4∗A15 + 8∗A10 + 2∗A12 + 3∗A19 + A125 + A1 + A118 + A16 + A22∗D22 + A30∗D30	27.40	0	63.34	75.7	27.40	32.7	[47]
$C_{16}H_{14}O_3$ ((±) α-(3-benzoylphenyl)priopinic acid (ketoprofen))	369.0	9∗A10 + A11 + 2∗A12 + A35 + A36∗B36 + A1 + A3∗B3	25.04	0	67.86	70.6	25.0	26.0	[200]
$C_{16}H_{14}O_4$ (5,6-dicarbomethoxy-acenaphthene)	450.2	4∗A10 + A14 + 2∗A15 + 3∗A19 + 2∗A1 + 3∗A12 + 2∗A38	34.73	0	77.14	61.6	34.73	27.7	[55]
$C_{16}H_{14}O_4$ (1,2-*cis*-dicarbomethoxy-acenaphthene)	398.2	6∗A10 + A14 + 2∗A15 + 3∗A19 + 2∗A1 + A12 + + 2∗A16 + 2∗A38	37.66	0	94.58	62.0	37.66	24.7	[55]
$C_{16}H_{14}O_4$ (1,2-*trans*-dicarbomethoxy-acenaphthene)	388.7	6∗A10 + A14 + 2∗A15 + 3∗A19 + 2∗A1 + A12 + + 2∗A16 + 2∗A38	27.61	0	71.03	62.0	27.61	24.1	[55]
$C_{16}H_{14}O_4$ (1,5-dicarbomethoxy-acenaphthene)	386.7	5∗A10 + A14 + 2∗A15 + 3∗A19 + 2∗A1 + 2∗A12 + + A16 + 2∗A38	28.87	0	74.66	61.90	28.87	23.9	[55]
$C_{16}H_{14}O_4$ (1,3-dicarbomethoxy-acenaphthene)	371.2	5∗A10 + A14 + 2∗A15 + 3∗A19 + 2∗A1 + 2∗A12 + + A16 + 2∗A38	23.01	0	61.99	61.90	23.01	22.9	[55]
$C_{16}H_{15}IO_3S$ (4-(4-pentenyloxy)phenyl-5-iodo-2-thiophene carboxylate)	332.7	A14 + 2*A15 + 4*A10 + 2*A12 + A5 + A6 + 2*A18 + 2*A19 + A131 + A29 + A32 + A38 + 3*A2 (not used in generating the statistics; experimental values in this article appear significantly out of line with both related molecules and estimations)	68.20	0	205.0	106.2	68.20	35.3	[230]
$C_{16}H_{15}N_5O_3$ (6-phenyl-3,9-dihydro-3-[(2-hydroxyethoxy)methyl]-9-oxo-5*H*-imidazol[1,2a]pyrine)	485.8	5∗A10 + A12 + 3∗A14 + 3∗A15 + 3∗A2 + A32 + 2∗A18∗B18 + 4∗A19 + A125 + A121 + 2∗A118 + A119 + A30∗E30	63.78	0	131.3	94.2	63.78	45.8	[31]

$C_{16}H_{16}$ (1,1-di-(4-methylphenyl)ethene)	334.1	8∗A10 + 2∗A12 + 2∗A11 + 2∗A1 + A7 + A5	23.31	0	69.77	66.8	23.31	22.3	[34]
$C_{16}H_{16}ClN$ (4-chlorobenzylidene-4′-propylaniline)	343.7	8∗A10 + 3∗A12 + A11 + A6∗B6 + A42 + A22∗B22 + A1 + 2∗A2 + 2∗A1 + 2∗A32 + 8∗A10 + 4∗A12 + A54 + A6∗B6	24.61	0	71.60	77.3	24.61	26.6	[219]
$C_{16}H_{17}F$ (2-fluoro-2-methyl-1, 3-diphenylpropane)	332.7	10∗A10 + 2∗A11 + A1 + 2∗A2 + A27 + A4∗B4	29.70	0	89.27	76.33	29.70	25.39	[95]
$C_{16}H_{19}NO$ (2-(4-butoxyphenyl)-5-methylpyridine)	363	7∗A10 + 4∗A12 + A1 + A32 + A41 + 3∗A2	33.0	0	90.9	76.3	33.0	27.7	[199]
$C_{16}H_{20}O_2$ (2-isopropyl-6-(1-hydroperoxy-1-methylethyl)naphthalene)	335.2	6∗A10 + 4∗A1 + 2∗A11 + 2∗A12 + A3 + A4∗B4 + A158	24.9	0	74.28	73.0	24.9	24.5	[135]
$C_{16}H_{20}O_4$ (2,6-bis-(1-hydroperoxy-1-methylethyl)naphthalene)	394.2	6∗A10 + 4∗A1 + 2∗A11 + 2∗A12 + 2∗A4∗B4 + 2∗A158	38.3	0	97.16	98.3	38.3	38.7	[135]
$C_{16}H_{21}NO_2$ ((−) 1-(isopropylamino)-3-(1-naphthyloxy)-2-propanol (propranolol))	344.7	7∗A10 + 2∗A1 + 3∗A12 + 2∗A2 + 2∗A3∗B3 + A44 + A32 + A30∗C30	36.25	0	105.2	74.9	36.25	25.8	[71]
$C_{16}H_{21}NO_2$ ((±) 1-(isopropylamino)-3-(1-naphthyloxy)-2-propanol (propranolol))	365.5	7∗A10 + 2∗A1 + 3∗A12 + 2∗A2 + 2∗A3∗B3 + A44 + A32 + A30∗C30	43.45	0	118.9	74.9	43.45	27.4	[71]
$C_{16}H_{24}N_2$ (2-(4-*tert*-butylphenyl)-2-(diethylamino)acetonitrile)	327.2	5∗A1 + 2∗A2 + 4∗A10 + 2∗A12 + A4 + A3∗B3 + A43 + A56	24.39	0	74.54	63.5	24.39	20.8	[87]
$C_{16}H_{24}N_2O$ (*N*-(2,6-dimethylphenyl)-1-ethyl-2-piperidinecarboxamide)	408.2	3∗A1 + 3∗A10 + 2∗A11 + A12 + A14 + 3∗A15 + A61 + 2∗A16 + A119 + A2	19.90	0	48.75	79.1	19.90	32.3	[139]
$C_{16}H_{24}N_2O_4$ (nonyl-*N*-(4-nitrophenyl) carbamate)	378.6	A1 + 8∗A2 + A69 + 4∗A10 + 2∗A12 + A50	37.00	0	97.72	114.4	37.00	43.3	[114]
$C_{16}H_{30}O_2$ (*cis*-9-hexadecenoic acid (palmitoleic acid))	254.8	A1 + 2∗A6 + A36 + 12∗A2∗B2	7.5	29.43					[217]
	275.2		32.1	116.6	146.1	153.2	39.6	42.2	
$C_{16}H_{34}O_2$ (1,16-hexadecanediol)	365.4	2∗A30∗B30 + 16∗A2∗B2	64.2	0	175.7	184.2	64.20	67.3	[15]
$C_{16}H_{34}O_4S_2$ (2-deoxy-D-glucose dipentyl dithioacetal)	393.3	2∗A1 + 10∗A2 + 4∗A3∗B3 + 2∗A84 + 4∗A30∗F30	63.1	0	160.4	160.1	63.1	63.0	[238]
$C_{16}H_{34}O_5S_2$ (D-glucose dipentyl dithioacetal)	389.0	2∗A1 + 9∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	49.1	0	126.0	165.5	49.1	64.4	[238]
$C_{16}H_{34}O_5S_2$ (L-rhamnose dipentyl dithioacetal)	388.2	2∗A1 + 9∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	46.5	0	119.8	165.5	46.5	64.3	[238]
$C_{16}H_{34}O_5S_2$ (L-arabinose dipentyl dithioacetal)	368.0	2∗A1 + 9∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	37.3	0	101.4	165.5	37.3	60.9	[238]
$C_{16}H_{34}O_5S_2$ (D-galactose dipentyl dithioacetal)	384.6	2∗A1 + 9∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	2.7	7.02					[238]
	392.1		41.1	104.8	111.8	165.5	43.8	64.9	

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{17}H_{15}NO_3S$ (4-(4-pentenyloxy)-phenyl-5-cyano-2-thiophene carboxylate)	337.6	A14 + 2∗A15 + 4∗A10 + 2∗A12 + A5 + A6 + 2∗A18 + 2∗A19 + A131 + A56 + A32 + A38 + 3∗A2 (not used in generating the statistics; experimental values in this article appear significantly out of line with both related molecules and estimations)	72.80	0	215.6	104.5	72.80	35.3	[230]
$C_{17}H_{17}N_5O_4$ (6-(4-methoxyphenyl)-3, 9-dihydro-3-[(2-hydroxyethoxy)-methyl]-9-oxo-5*H*-imidazol [1,2-a]pyrine)	507.3	4∗A10 + 2∗A12 + 3∗A14 + 3∗A15 + 3∗A2 + A1 + 2∗A32 + 2∗A18∗B18 + 4∗A19 + A125 + A121 + 2∗A118 + A119 + A30∗F30	48.41	0	95.43	103.4	48.41	52.4	[31]
$C_{17}H_{18}O_4$ (2-hydroxy-4, 4′-diethoxybenzophenone)	373.6	7∗A10 + 5∗A12 + A35 + A31 + 2∗A1 + 2∗A32 + 2∗A2	34.7	0	92.88	98.0	34.7	36.6	[136]
$C_{17}H_{18}O_4S$ (4-(4-pentenyloxy)phenyl-5-methoxy-2-thiophene carboxylate)	333.7	A14 + 2∗A15 + 4∗A10 + 2∗A12 + A5 + A6 + 2∗A18 + 2∗A19 + A131 + A1 + 2∗A32 + A38 + 3∗A2 (not used in generating the statistics; experimental values in this article appear significantly out of line with both related molecules and estimations)	74.48	0	223.2	109.1	74.48	36.4	[228]
$C_{17}H_{20}O_2$ (diethoxydiphenylmethane)	323.2	10∗A10 + 2∗A11 + 2∗A1 + 2∗A2 + A4∗B4 + 2∗A32	19.9	0	61.55	90.7	19.9	29.3	[88]
$C_{17}H_{22}O_3S$ (*p*-(1*R*,3*S*)-3-thianisoyl-1,2, 2-trimethylcyclopentanecarboxylic acid)	393.7	4∗A10 + 2∗A12 + 4∗A1 + A84 + A35 + A14 + 2∗A15 + A36∗C36 + 2∗A17 + A16	23.56	0	59.84	78.8	23.56	31.0	[58,59]
$C_{17}H_{26}N_2O$ (*N*-(2,6-dimethylphenyl)-1-propyl-2-piperidinecarboxamide)	414.2	3∗A1 + 3∗A10 + 2∗A11 + A12 + A14 + 3∗A15 + A61 + 2∗A16 + A119 + 2∗A2	44.50	0	107.4	86.2	44.50	35.7	[139]
$C_{17}H_{27}N_3O_3$ (1-decyl-3-(4-nitrophenyl) urea)	390.6	A1 + 9∗A2∗B2 + A66 + 4∗A10 + 2∗A12 + A50	37.92	0	97.08	135.1	37.92	52.8	[114]
$C_{17}H_{36}O_2$ (1,17-heptadecanediol)	354.6	2∗A30∗B30 + 17∗A2∗B2	34.90	98.4					[15]
	367.3		30.80	83.9	182.3	193.5	65.70	71.0	
$C_{18}H_{14}$ (*m*-terphenyl)	361.2	14∗A10 + 4∗A12 (compound is already in database, however, this experimental value is significantly different than the previous one)	31.00	0	85.83	73.6	31.00	26.6	[96]

$C_{18}H_{16}N_2O_2$ (*meso*-2,3-dimethoxy-2,3-diphenylsuccinonitrile)	469.7	10∗A10 + 2∗A11 + 2∗A1 + 2∗A32 + 2∗A4∗B4 + 2∗A56	25.10	0	53.4	88.9	25.10	41.7	[169]
$C_{18}H_{18}ClNS$ (3-(2-chloro-9*H*-thioxanthen-9-ylidene)-*N*,*N*-dimethyl-1-propanamine (2-chlorprothixene))	370.5	A14 + 3∗A15 + 7∗A10 + 2∗A1 + 2∗A2 + 5∗A19 + A6 + A43 + A131 + A22∗C22	28.90	0	78.00	86.4	28.90	32.0	[235]
$C_{18}H_{18}O_2$ (3-(diphenylmethyl)-2,4-pentanedione)	387.2	2∗A1 + A3 + A3∗B3 + 10∗A10 + 2∗A11 + 2∗A35	27.02	0	69.78	73.0	27.02	28.3	[84]
$C_{18}H_{18}O_4$ (2,2′-diphenyl-bi(1,3-dioxolan-2-yl))	456.1	2∗A14 + 4∗A15 + 2∗A17 + 4∗A112 + 10∗A10 + 2∗A11	32.1	0	70.38	73.0	32.1	28.3	[216]
$C_{18}H_{19}Cl_2NO_4$ (ethyl methyl-4-(2,3-dichlorophenyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate (felodipine))	414.9	3∗A10 + 2∗A12 + A11 + A14 + 3∗A15 + 4∗A1 + 4∗A19 + A16 + 2∗A38 + 2∗A22∗F22 + A121 + A2	35.21	0	84.86	105.7	35.2	43.9	[217]
$C_{18}H_{19}N$ ((*S*) 4-(2-methylbutyl)-4′-cyanobiphenyl)	276.0	2∗A1 + 2∗A2 + A3 + 8∗A10 + A11 + 3∗A12 + A56 (compound may have phase transitions at lower temperatures)	10.7	0	38.8	77.8	10.7	21.5	[171]
$C_{18}H_{20}BrN_5O_5$ (8-bromo-(*R*)-7-[2-hydroxy-3-(4-acetylamino)-fenoxypropyl]-1,3-dimethylxanthine)	492.2	2∗A14 + 3∗A15 + 2∗A59 + 3∗A19 + A119 + A118 + 3∗A1 + 2∗A2 + A3∗B3 + A32 + A30∗F30 + 4∗A10 + 2∗A12 + A60 + A21	37.8	0	76.8	117.5	37.8	57.9	[77]
$C_{18}H_{20}N_2O_6$ (3-ethyl-5-methyl-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylate ((*RS*)-nitrendipine))	430.7	A14 + 3∗A15 + 4∗A10 + A11 + A12 + 4∗A19 + A16 + 4∗A1 + A2 + A50 + 2∗A38 + A121	41.1	0	95.43	105.9	41.1	45.6	[231]
$C_{18}H_{20}N_6O_7$ (8-nitro-(*R*)-7-[2-hydroxy-3-(4-acetylamino)-fenoxypropyl]-1,3-dimethylxanthine)	481.2	2∗A14 + 3∗A15 + 2∗A59 + 3∗A19 + A119 + A118 + 3∗A1 + 2∗A2 + A3∗B3 + A32 + A30∗F30 + 4∗A10 + 2∗A12 + A60 + A50	56.8	0	118.0	117.7	56.8	56.7	[77]
$C_{18}H_{20}O_4$ (2-hydroxy-4-butoxy-4′-methoxybenzophenone)	345.6	7∗A10 + 5∗A12 + A35 + A31 + 2∗A1 + 2∗A32 + 3∗A2	33.7	0	97.51	105.1	33.7	36.3	[136]
$C_{18}H_{21}N_5O_5$ ((*R*)-7-[2-hydroxy-3-(4-acetylamino)-fenoxypropyl]-1,3-dimethylxanthine)	477.2	2∗A14 + 3∗A15 + 2∗A59 + 2∗A19 + A18∗B18 + A119 + A118 + 3∗A1 + 2∗A2 + A3∗B3 + A32 + A30∗F30 + 4∗A10 + 2∗A12 + A60	65.9	0	138.1	109.3	65.9	52.1	[77]
$C_{18}H_{22}O_4$ (1,2-diphenyl-1,1,2,2-tetramethoxyethane)	328.5	4∗A1 + 10∗A10 + 2∗A11 + 4∗A32 + 2∗A4∗B4	20.1	0	61.18	98.1	20.1	32.1	[131]
$C_{18}H_{24}$ ((E)-9-(bicyclo[4.2.1]non-3-en-9-ylidene)bicyclo[4.2.1]non-3-ene)	441.7	4∗A14 + 6∗A15 + 4∗A16 + 4∗A18 + 2∗A19	9.10	0	20.60	66.0	9.10	29.2	[75]
$C_{18}H_{24}$ ((Z)-9-(bicyclo[4.2.1]non-3-en-9-ylidene)bicyclo[4.2.1]non-3-ene)	440.8	4∗A14 + 6∗A15 + 4∗A16 + 4∗A18 + 2∗A19	27.96	0	64.33	66.0	27.96	29.1	[75]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{18}H_{24}N_2O_4$ ((4-nitrophenyl)-10-undecynyl carbamate)	385.4	9∗A2 + A8 + A9 + 4∗A10 + 2∗A12 + A50 + A69	53.18	0	138.0	118.9	53.18	44.7	[114]
$C_{18}H_{24}O$ ((1*R*,1″*R*,6*S*,6″*S*,9*S*,9″*S*)-dispiro(bicyclo[4.2.1]non-3-ene-9,2′-oxirane-3′,9″-bicyclo[4.2.1]non-3-ene))	354.3	5∗A14 + 4∗A15 + 4∗A16 + 2∗A17 + 4∗A18 + A112	5.92	16.85					[75]
	373.8		8.19	21.86	38.71	48.6	14.11	18.2	
$C_{18}H_{24}O$ ((1*R*,1″*R*,6*S*,6″*S*,9*R*,9″*S*)-dispiro(bicyclo[4.2.1]non-3-ene-9,2′-oxirane-3′,9″-bicyclo[4.2.1]non-3-ene))	333.9	5∗A14 + 4∗A15 + 4∗A16 + 2∗A17 + 4∗A18 + A112	14.92	0	44.60	48.6	14.92	16.2	[75]
$C_{18}H_{26}N_2O_4$ ((4-nitrophenyl)-10-undecenyl carbamate)	376.4	9∗A2 + A5 + A6 + 4∗A10 + 2∗A12 + A50 + A69	43.81	0	116.4	126.5	43.81	47.6	[114]
$C_{18}H_{27}BrN_2O_4$ ((4-nitrophenyl)-11-bromoundecyl carbamate)	395.6	11∗A2∗B2 + A69 + 4∗A10 + 2∗A12 + A50 + A21	58.56	0	148.0	159.8	58.56	63.2	[114]
$C_{18}H_{27}IN_2O_4$ ((4-nitrophenyl)-11-iodoundecyl carbamate)	399.6	11∗A2∗B2 + A69 + 4∗A10 + 2∗A12 + A50 + A29	63.34	0	158.5	161.7	63.34	64.6	[114]
$C_{18}H_{28}$ ((E)-9-(bicyclo[4.2.1]nonan-9-ylidene)bicyclo[4.2.1]nonane)	224.8	4∗A14 + 6∗A15 + 4∗A16 + 2∗A19	2.68	11.92					[75]
	412.4		9.32	22.61	34.53	72.4	12.0	29.9	
$C_{18}H_{28}$ ((Z)-9-(bicyclo[4.2.1]nonan-9-ylidene)bicyclo[4.2.1]nonane)	344.3	4∗A14 + 6∗A15 + 4∗A16 + 2∗A19	10.12	29.39					[75]
	393.3		11.04	28.15	57.54	72.4	21.16	28.5	
$C_{18}H_{28}N_2O$ (*N*-(2,6-dimethylphenyl)-1-butyl-2-piperidinecarboxamide)	413.2	3∗A1 + 3∗A10 + 2∗A11 + A12 + A14 + 3∗A15 + A61 + 2∗A16 + A119 + 3∗A2	26.25	0	63.53	93.3	26.25	38.6	[139]
$C_{18}H_{28}O$ ((1*R*,1″*R*,6*S*,6″*S*,9*R*,9″*R*)-dispiro(bicyclo[4.2.1]nonane-9,2′-oxirane-3′,9″-bicyclo-[4.2.1]nonane))	348.5	5∗A14 + 4∗A15 + 4∗A16 + 2∗A17 + A112	9.74	27.92					[75]
	444.1		13.13	29.55	57.57	55.0	22.87	24.4	
$C_{18}H_{28}O$ ((1*R*,1″*R*,6*S*,6″*S*,9*R*,9″*S*)-dispiro(bicyclo[4.2.1]nonane-9,2′-oxirane-3′,9″-bicyclo[4.2.1]nonane))	274.9	5∗A14 + 4∗A15 + 4∗A16 + 2∗A17 + A112	0.72	2.59					[75]
	342.5		6.35	18.52	21.11	55.0	7.07	18.8	
$C_{18}H_{29}NO_2$ (2,4,6-tri-*tert*-butylnitrobenzene)	482.8	2∗A10 + A12 + 3∗A11 + 9∗A1 + 3∗A4 + A50	19.25	0	39.87	50.2	19.25	24.2	[230]
$C_{18}H_{30}$ (1-phenyldodecane)	274.6	5∗A10 + A11 + A1 + 11∗A2∗B2	43.1	0	157.0	147.3	43.1	40.5	[148]
$C_{18}H_{31}N$ (2,4,6-tri-*tert*-butylaniline)	426.4	9∗A1 + 3∗A4 + 2∗A10 + A12 + 3∗A11 + A45	19.38	0	45.45	53.9	19.38	23.0	[105]

$C_{18}H_{34}$ (1,4-diphenylbicyclo[2.2.2]octane)	261.5	2∗A14 + 2∗A15 + 2∗A17 + 10∗A10 + 2∗A11	20.4	0	78.01	59.8	20.4	15.6	[127]
$C_{18}H_{34}O_2$ (*cis*-11-octadecenoic acid (asclepic acid))	257.8	A1 + 14∗A2∗B2 + 2∗A6 + A36	7.8	30.26					[217]
	287.0		39.8	138.7	168.9	171.8	47.6	49.3	
$C_{18}H_{36}N_2$ (tetraisobutylsuccinonitrile)	360.2	8∗A1 + 2∗A4∗B4 + 4∗A2 + 4∗A3 + 2∗A56	34.31	0	95.25	93.1	34.31	33.5	[168]
$C_{18}H_{36}O_2$ (ethyl hexadecanoate)	296.0	2∗A1 + A38 + 14∗A2∗B2 + A2	53.14	0	179.5	180.6	53.14	53.3	[92]
$C_{18}H_{38}O_2$ (1,18-octadecanediol)	366.1	2∗A30∗B30 + 18∗A2∗B2	38.70	105.7					[15]
	371.5		33.60	90.4	196.1	202.7	72.30	75.3	
$C_{18}H_{38}O_4S_2$ (2-deoxy-D-glucose dihexyl dithioacetal)	376.2	2∗A1 + 12∗A2 + 4∗A3∗B3 + 2∗A84 + 4∗A30∗F30	16.4	43.6					[218]
	386.4		45.0	116.5	160.1	174.3	61.4	67.4	
$C_{18}H_{38}O_4$ (6,6′-[1,6-hexanediylbis(oxy)]bis-1-hexanol)	329.1	18∗A2∗B2 + 2∗A30∗E30 + 2∗A32	57.96	0	176.1	221.4	57.96	72.9	[109]
$C_{18}H_{38}O_5S_2$ (D-glucose dihexyl dithioacetal)	373.6	2∗A1 + 11∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	5.9	15.79					[238]
	377.0		44.6	118.3	134.1	179.7	50.5	67.7	
$C_{18}H_{38}O_5S_2$ (L-rhamnose dihexyl dithioacetal)	388.2	2∗A1 + 11∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	48.5	0	124.9	179.7	48.5	69.7	[238]
$C_{18}H_{38}O_5S_2$ (L-arabinose dihexyl dithioacetal)	345.1	2∗A1 + 11∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	6.7	19.41					[238]
	358.2		1.0	2.80					
	367.2		39.2	106.8	129.0	179.7	46.9	66.0	
$C_{19}H_{14}O_4$ (4-hydroxyphenyl-4″-hydroxybiphenyl-4′-carboxylate)	566.2	12∗A10 + 6A12 + 2∗A31 + A38	49.59	0	87.58	92.1	49.49	52.15	[184]
$C_{19}H_{15}F_9OS$ (4-[[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)thio]methoxy]-1,1′-biphenyl)	333.3	9∗A10 + 2∗A12 + A11 + A84 + 3∗A2 + A32 + 3∗A25 + 6∗A26∗C26 + 4∗A4∗B4	43.1	0	129.3	104.2	43.1	34.7	[16]
$C_{19}H_{15}F_9S$ (4-[[(3,3,4,4,5,5,6,6,6-nonafluorohexyl)thio]methyl]-1,1′-biphenyl)	307.1	9∗A10 + 2∗A12 + A11 + A84 + 3∗A2 + 3∗A25 + 6∗A26∗B26 + 4∗A4∗B4	41.0	0	133.5	97.4	41.0	29.9	[16]
$C_{19}H_{16}ClNO_4$ (1-(4-chlorobenzyl)-5-methoxy-2-methyl-1*H*-indole-3-acetic acid (indomethacin))	435.2	A14 + 2∗A15 + 4∗A19 + A146 + 7∗A10 + 3∗A12 + A22∗E22 + A32 + A36∗E36 + 2∗A1 + A2	36.49	0	83.85	105.3	36.49	45.8	[183]
$C_{19}H_{16}O$ (triphenylcarbinol)	441.1	15∗A10 + 3∗A11 + A30 + A4∗B4	27.24	0	61.75	60.9	27.24	26.9	[72]
$C_{19}H_{16}O_2$ (2-fluorenyl-2-methyl-1,3-cyclopentanedione)	395.2	2∗A14 + 4∗A15 + 8∗A10 + 4∗A19 + A16 + A1 + A17 + 2∗A114	24.6	0	62.25	57.1	24.6	22.6	[84]
$C_{19}H_{18}FNO_3$ (4-cyano-2-fluorophenyl-4-pentoxybenzoate)	359.7	7∗A10 + 5∗A12 + A24 + A56 + A38 + A1 + 4∗A2 + A32	36.2	0	100.6	107.0	36.2	38.5	[239]
$C_{19}H_{18}FNO_3$ (4-cyano-3-fluorophenyl-4-pentoxybenzoate)	341.2	7∗A10 + 5∗A12 + A24 + A56 + A38 + A1 + 4∗A2 + A32	37.7	0	110.5	107.0	37.7	36.5	[239]
$C_{19}H_{18}O_2$ (2-(diphenylmethyl)-2-methyl-1,3-cyclopentanedione)	394.2	A14 + 2∗A15 + 10∗A10 + 2∗A11 + A1 + A3 + A17 + 2∗A114	34.3	0	87.01	59.4	34.3	23.4	[84]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{19}H_{20}O_3$ (1-(diphenylmethyl)-4-methyl-2,6,7-trioxabicyclo-[2.2.2]octane)	443.2	2∗A14 + 2∗A15 + 3∗A112 + A1 + 2∗A17 + 10∗A10 + 2∗A11 + A3	32.6	0	73.56	64.6	32.6	28.6	[86]
$C_{19}H_{21}IO_3S$ (4-(7-octenyloxy)-phenyl-5-iodo-2-thiophene carboxylate)	324.9	A14 + 2∗A15 + 4∗A10 + 2∗A12 + A5 + A6 + 2∗A18 + 2∗A19 + A131 + A29 + A32 + A38 + 6∗A2 (not used in generating the statistics; experimental values in this article appear significantly out of line with both related molecules and estimations)	80.33	0	247.2	127.5	80.33	41.43	[228]
$C_{19}H_{22}FN_3O$ (1-(4-fluorophenyl)-4-[4-(2-pyridinyl)-1-piperazinyl]-1-butanone (azaperone))	366.2	A14 + 3∗A15 + 2∗A119 + A35 + A24 + 8∗A10 + 3∗A12 + 3∗A2 + A41	30.5	0	83.3	96.0	30.5	35.2	[205]
$C_{19}H_{24}N_2O_2$ ((±) 2-(cyclohexylcarbonyl)-1,2,3,6,7,11b-hexahydro-4*H*-pyrazino[2,1a]-isoquinolin-4-one ((±) praziquantel))	412.2	4∗A10 + 3∗A14 + 7∗A15 + 2∗A19 + 2∗A16 + A125 + A146	30.80	0	74.72	71.0	30.80	29.3	[236]
$C_{19}H_{24}N_2O_2$ ((+) 2-(cyclohexylcarbonyl)-1,2,3,6,7,11b-hexahydro-4*H*-pyrazino[2,1a]isoquinolin-4-one ((+) praziquantel))	386.0	4∗A10 + 3∗A14 + 7∗A15 + 2∗A19 + 2∗A16 + A125 + A146	23.90	0	61.92	71.0	23.90	27.4	[236]
$C_{19}H_{24}N_2O_2$ ((−) 2-(cyclohexylcarbonyl)-1,2,3,6,7,11b-hexahydro-4*H*-pyrazino[2,1a]isoquinolin-4-one ((−) praziquantel))	385.5	4∗A10 + 3∗A14 + 7∗A15 + 2∗A19 + 2∗A16 + A125 + A146	24.15	0	62.64	71.0	24.15	27.4	[236]
$C_{19}H_{27}NO_4$ (β-cyano-3,4-dimethoxy-α,α-dimethyl-β-(1-methylethyl)-benzenepropanoic acid ethyl ester)	386.2	3∗A10 + 2∗A12 + A11 + 7∗A1 + A2 + 2∗A4 + A3 + A56 + 2∗A32 + A38	38.82	0	95.34	100.4	36.82	38.8	[222]
$C_{19}H_{29}BrN_2O_4$ ((4-nitrophenyl)-12-bromododecyl carbamate)	373.5	12∗A2∗B2 + A69 + 4∗A10 + 2∗A12 + A50 + A21	48.94	0	131.0	169.1	48.94	63.2	[114]
$C_{19}H_{31}N_3O_3$ (1-dodecyl-3-(4-nitrophenyl) urea)	390.8	A1 + 11∗A2∗B2 + A66 + 4∗A10 + 2∗A12 + A50	40.88	0	104.6	153.7	40.88	60.1	[114]
$C_{19}H_{38}O$ (2-nonadecanone)	333.9	2∗A1 + A35 + 16∗A2∗B2	70.0	0	209.7	188.7	70.0	63.0	[144]
$C_{19}H_{38}O$ (10-nonadecanone)	330.0	2∗A1 + A35 + 16∗A2∗B2	66.1	0	200.3	188.7	66.1	62.2	[144]
$C_{19}H_{40}O_2$ (1,19-nonadecanediol)	358.9	2∗A30∗B30 + 19∗A2∗B2	37.10	103.4					[15]
	373.9		35.70	95.5	198.9	212.1	72.80	79.3	

$C_{20}H_{13}N_5O_3$ (1-(2′-nitrobenzylidene)-2-phenazinoylhydrazine)	540.2	11∗A10 + 7∗A12 + 2∗A41 + A6∗B6 + A50 + A159	47.47	0	87.9	91.0	47.47	49.1	[29]
$C_{20}H_{13}N_5O_3$ (1-(4′-nitrobenzylidene)-2-phenazinoylhydrazine)	548.2	11∗A10 + 7∗A12 + 2∗A41 + A6∗B6 + A50 + A159	44.80	0	81.7	91.0	44.80	49.9	[29]
$C_{20}H_{14}N_4O$ (1-benzylidene-2-phenazinoylhydrazine)	512.1	12∗A10 + 6∗A12 + 2∗A41 + A6∗B6 + A159	45.76	0	94.6	88.2	45.76	45.1	[29]
$C_{20}H_{15}BrN_4O_6$ (3,5-dinitro-4-(4-methoxyphenyl)aminobenzoyl (4-bromophenyl)amide)	522.5	A1 + 10∗A10 + 8∗A12 + A32 + A44 + A21 + 2∗A50 + A60	50.67	0	96.98	85.4	50.67	44.6	[149]
$C_{20}H_{15}BrN_4O_6$ (3,5-dinitro-2-(4-methoxyphenyl)aminobenzoyl (4-bromophenyl)amide)	478.9	A1 + 10∗A10 + 8∗A12 + A32 + A44 + A21 + 2∗A50 + A60	38.00	0	79.35	85.4	38.00	40.9	[149]
$C_{20}H_{15}F_3$ (1,1,1-trifluoro-2,2,2-triphenylethane)	440.3	15∗A10 + 3∗A11 + A4 + A4∗B4 + 3∗A25	30.33	0	68.88	64.3	30.33	28.3	[95]
$C_{20}H_{15}O_5P$ (bis(4-carboxyphenyl)-phenylphosphine oxide)	610.6	13∗A10 + 5∗A12 + 2∗A36∗C36 + A73	17.6	0	28.82	86.3	17.6	52.6	[178]
$C_{20}H_{16}$ (triphenylethene)	341.0	15∗A10 + 3∗A12 + A6 + A7	20.35	0	59.67	83.1	20.35	28.3	[49]
$C_{20}H_{17}N_5O_3$ (6-(2-naphthyl)-3,9-dihydro-3-[(2-hydroxyethoxy)-methyl]-9-oxo-5*H*-imidazol[1,2a]pyrine)	493.4	7∗A10 + 3∗A12 + 3∗A14 + 3∗A15 + 3∗A2 + A32 + 2∗A18∗B18 + 4∗A19 + A125 + A121 + 2∗A118 + A119 + A30∗E30	37.64	0	76.29	94.0	37.64	46.4	[31]
$C_{20}H_{18}$ (1,1,2-triphenylethane)	328.2	15∗A10 + 3∗A11 + A2 + A3	24.39	0	74.31	89.9	24.39	29.5	[40]
$C_{20}H_{18}$ (1,1,1-triphenylethane)	375.9	15∗A10 + 3∗A11 + A1 + A4	19.95	0	53.07	65.0	19.95	24.4	[40]
$C_{20}H_{18}O_2$ (2-fluorenyl-2-methyl-1,3-cyclohexanedione)	448.2	2∗A14 + 5∗A15 + 8∗A10 + 4∗A19 + A16 + A1 + A17 + 2∗A114	35.7	0	79.65	60.8	35.7	27.3	[84]
$C_{20}H_{18}O_6$ (9-fluorenyltris-(methoxycarbonyl)methane)	407.2	A14 + 2∗A15 + 8∗A10 + 4∗A19 + A16 + 3∗A1 + 3∗A38 + A4∗B4	32.3	0	79.32	89.0	32.3	36.3	[85]
$C_{20}H_{20}FNO_3$ (4-cyano-3-fluorophenyl-4-hexyloxybenzoate)	332.7	7∗A10 + 5∗A12 + A24 + A56 + A38 + A1 + 5∗A2 + A32	35.56	0	106.9	114.1	35.6	38.0	[239]
$C_{20}H_{20}O_2$ (2-(diphenylmethyl)-2-ethyl-1,3-cyclopentanedione)	382.2	A14 + 2∗A15 + 10∗A10 + 2∗A11 + A1 + A2 + A3 + A17 + 2∗A114	28.2	0	73.78	66.5	28.2	25.4	[84]
$C_{20}H_{20}O_6$ (1,1,1-tris(methoxycarbonyl)-2,2-diphenylethane)	414.2	3∗A1 + 10∗A10 + 2∗A11 + A3 + A4 + 3∗A38	36.1	0	87.16	91.3	36.1	37.8	[85]
$C_{20}H_{21}NO_3S$ (4-(7-octenyloxy)phenyl-5-cyano-2-thiophene carboxylate)	332.7	A14 + 2∗A15 + 4∗A10 + 2∗A12 + A5 + A6 + 2∗A18 + 2∗A19 + A131 + A56 + A32 + A38 + 6∗A2 (not used in generating the statistics; experimental values in this article appear significantly out of line with both related molecules and estimations)	68.20	0	205.0	125.0	68.20	41.85	[228]
$C_{20}H_{21}N_3O_5S$ (2-methyl-1,1-dioxido-3-[(2-pyridinylamino)carbonyl]-2*H*-1,2-benzothiazin-4-yl-2,2-dimethylpropanoic acid ester (piroxicam pivalate))	427.0	Group values not available	32.74	0	76.67		32.74		[61]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{20}H_{21}O_4S$ (4-(7-octenyloxy)phenyl-5-methoxy-2-thiophene carboxylate)	332.8	A14 + 2∗A15 + 4∗A10 + 2∗A12 + A5 + A6 + 2∗A18 + 2∗A19 + A131 + A1 + 2∗A32 + A38 + 6∗A2 (not used in generating the statistics; experimental values in this article appear significantly out of line with both related molecules and estimations)	76.57	0	230.1	130.4	76.57	43.4	[230]
$C_{20}H_{22}O_2$ (3-(diphenylmethyl)-3-ethyl-2,4-pentanedione)	388.2	3∗A1 + A2 + A3 + A4 + 10∗A10 + 2∗A11 + 2∗A35	34.7	0	89.39	72.7	34.7	28.2	[84]
$C_{20}H_{23}FN_2O$ (1-(4-fluorophenyl)-4-[4-phenyl-1-piperazinyl]-1-butanone (butropipazone))									
Form I	387.2	A14 + 3∗A15 + 2∗A119 + A35 + A24 + 9∗A10 + 3∗A12 + 3∗A2	36.7	0	94.8	92.5	36.7	35.8	[205]
Form II	363.7		34.7	0	95.4	92.5	34.7	33.6	
$C_{20}H_{27}NO_4$ ((−) 1-[[2-(3,4-dimethoxyphenyl)ethyl]-amino]-3-(3-methyl-phenoxy)-2-propanol (bevantolol))	348.3	3∗A1 + 4∗A2 + 7∗A10 + 2∗A11 + 3∗A12 + A44 + 3∗A32 + A30∗E30 + A3∗B3	43.22	0	124.1	101.6	43.22	38.6	[71]
$C_{20}H_{27}NO_4$ ((+) 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(3-methyl-phenoxy)-2-propanol (bevantolol))	360.6	3∗A1 + 4∗A2 + 7∗A10 + 2∗A11 + 3∗A12 + A44 + A32 + A30∗E30 + A3∗B3	45.90	0	127.3	101.6	45.90	40.0	[71]
$C_{20}H_{28}N_2$ (1-(4-cyanophenyl)-4-*n*-heptypiperidine)	326.2	A14 + 3∗A15 + A16 + A119 + 6∗A2 + A1 + 4∗A10 + A11 + A12 + A56	30.2	0	92.6	100.9	30.2	32.9	[240]
$C_{20}H_{34}AuO_9PS$ (5-triethylphospine gold-2,3,4,6-tetra-*O*-acetyl-1-thio-β-D-glucopyranoside (auranofin))	385.0	Group values not available	37.82	0	98.23		37.82		[134]
$C_{20}H_{38}O_2$ (*cis*-11-eicosenoic acid (gondoic acid))	270.0	A1 + 16∗A2∗B2 + 2∗A6 + A36	9.0	33.33					[217]
	296.5		49.7	167.6	200.9	190.4	58.7	56.5	
$C_{20}H_{40}O_2$ (ethyl octadecanoate)	307.0	2∗A1 + A38 + 16∗A2∗B2 + A2	59.83	0	194.9	198.8	59.83	61.0	[92]
$C_{20}H_{42}O_2$ (1,20-eicosanediol)	368.6	2∗A30∗B30 + 20∗A2∗B2	37.00	100.4					[15]
	376.1		39.70	105.6	206.0	221.3	76.70	83.2	
$C_{21}H_{13}F_{13}OS$ (2-(perfluoro-*n*-hexyl)ethylthiomethyl biphenyl-4-yl ether)	344.8	9∗A10 + 3∗A12 + A84 + 3∗A2 + A32 + 3∗A25 + 10∗A26∗C26 + 6∗A4∗B4	40.6	0	117.7	114.2	40.6	39.4	[16]
	344.8		40.4	0	117.2	114.2	40.4	47.6	[16,117]

$C_{21}H_{13}F_{13}S$ (2-(perfluoro-*n*-hexyl)ethylthiomethyl biphenyl-4-yl)	332.9	9∗A10 + 2∗A12 + A11 + A84 + 3∗A2 + 3∗A25 + 10∗A26∗B26 + 6∗A4∗B4	53.1	0	159.5	107.4	53.1	35.8	[16,117]
$C_{21}H_{16}N_4O_2$ (1-(4′-methoxybenzylidene)-2-phenazinoylhydrazine)	534.3	11∗A10 + 7∗A12 + 2∗A41 + A6∗B6 + A1 + A32 + A159	63.26	0	118.4	95.6	63.26	51.1	[29]
$C_{21}H_{18}F_2$ (1,1-difluoro-3,3,3-triphenylpropane)	370.2	15∗A10 + 3∗A11 + A2 + A4 + A3∗B3 + 2∗A26	28.74	0	71.1	77.46	28.74	26.3	[95]
$C_{21}H_{19}F$ (1-fluoro-3,3,3-triphenylpropane)	344.2	15∗A10 + 3∗A11 + A4 + 2∗A2 + A27	26.44	0	78.62	74.3	26.44	25.6	[95]
$C_{21}H_{19}F$ (2-fluoro-1,2,3-triphenylpropane)	379.6	15∗A10 + 3∗A11 + 2∗A2 + A27 + A4∗B4	34.60	0	91.15	86.1	34.60	32.7	[95]
$C_{21}H_{23}BrFNO_2$ (1-(4-fluorophenyl)-4-[4-hydroxy-4-(4-bromophenyl)-1-piperidinyl]-1-butanone (bromoperidol))	432.7	A14 + 3∗A15 + A17 + A119 + A30∗E30 + A35 + A24 + 8∗A10 + A11 + 3∗A12 + 3∗A2 + A21	50.8	0	117.4	98.3	50.8	42.5	[205]
$C_{21}H_{23}ClFNO_2$ (1-(4-fluorophenyl)-4-[4-hydroxy-4-(4-chlorophenyl)-1-piperidinyl]-1-butanone (haloperidol))	422.7	A14 + 3∗A15 + A17 + A119 + A30∗E30 + A35 + A24 + 8∗A10 + A11 + 3∗A12 + 3∗A2 + A22∗E22	48.0	0	113.6	97.0	48.0	41.0	[205]
$C_{21}H_{23}F_2NO_2$ (1-(4-fluorophenyl)-4-[4-hydroxy-4-(4-fluorophenyl)-1-piperidinyl]-1-butanone)	395.2	A14 + 3∗A15 + A17 + A119 + A30∗D30 + A35 + 2∗A24 + 8∗A10 + 4∗A12 + 3∗A2	34.0	0	86.0	101.2	34.0	40.0	[205]
$C_{21}H_{24}FNO_2$ (1-(4-fluorophenyl)-4-[4-hydroxy-4-phenyl-1-piperidinyl]-1-butanone)									
Form I	412.7	+ A14 + 3∗A15 + A17 + A119 + A30∗D30 + A35 + A24 + 9∗A10 + A11 + 2∗A12 + 3∗A2	43.2	0	104.7	97.4	43.2	40.2	[205]
Form II	385.2		35.2	0	91.4	97.4	35.2	37.5	
$C_{21}H_{24}O_2$ (3-(diphenylmethyl)-3-propyl-2,4-pentanedione)	349.2	3∗A1 + 2∗A2 + A3 + A4∗B4 + 10∗A10 + 2∗A11 + 2∗A35	27.1	0	77.61	91.6	27.1	32.0	[84]
$C_{21}H_{25}FN_2O_2$ (1-(4-fluorophenyl)-4-[4-(2-methoxyphenyl)-1-piperazinyl]-1-butanone (fluanizone))									
Form I	348.7	A14 + 3∗A15 + 2∗A119 + A35 + A24 + 8∗A10 + 4∗A12 + 3∗A2 + A1 + A32	27.3	0	78.3	99.1	27.3	34.8	[205]
Form II	343.7		31.1	0	90.5	99.1	31.1	34.3	
Form III	323.7		15.7	0	48.5	99.1	15.7	32.3	
$C_{21}H_{26}FNO$ (4-octyloxy-*N*-(4-fluorobenzylidene) aniline)	360.5	8∗A10 + 4∗A12 + A6∗B6 + A42 + 7∗A2 + A1 + A24 + A32	44.70	0	124	120.0	44.70	43.3	[220]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{21}H_{26}FN_3O_4$ ([*S*-(R^*,S^*)]-1-cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-7-[3-[1-(methylamino)ethyl]-1-pyrrolidinyl]-4-oxo-3-quinolinecarboxylic acid (premafloxacin))	471.9	3∗A14 + 5∗A15 + 3∗A1 + A10 + 3∗A12 + A32 + A44 + A16 + A24 + 2∗A119 + A114 + A18∗B18 + 3∗A19 + A36∗E36	60.52	0	128.2	83.3	60.52	39.3	[189]
$C_{21}H_{26}O_4$ (2-hydroxy-4, 4′-dibutoxybenzophenone)	372.1	7∗A10 + 5∗A12 + A35 + A31 + 2∗A1 + 2∗A32 + 6∗A2	54.0	0	145.1	126.4	54.0	47.0	[136]
$C_{21}H_{27}NO$ (4-octyloxy-*N*-benzylidene aniline)	342.7	9∗A10 + 3∗A12 + A6∗B6 + A42 + 7∗A2 + A1 + A32	41.47	0	121	118.3	41.47	40.5	[220]
$C_{21}H_{42}O_2$ (ethyl nonadecanoate)	309.0	2∗A1 + A38 + 17∗A2∗B2 + A2	43.10	0	139.5	208.1	43.10	64.3	[92]
$C_{21}H_{44}O_2$ (1,21-heneicosanediol)	360.0	2∗A30∗B30 + 21∗A2∗B2	38.80	107.8					[15]
	377.5		41.70	110.5	218.3	230.7	80.50	87.1	
$C_{21}H_{42}$ (*n*-pentadecylcyclohexane)	301	A14 + 3∗A15 + A1 + A16 + 14∗A2∗B2	58.3	0	193.7	177.6	58.3	53.5	[220]
$C_{22}H_{19}N_5O_3$ (6-(4-biphenylyl)-3, 9-dihydro-3-[(2-hydroxyethoxy)methyl]-9-oxo-5*H*-imidazol[1,2a]pyrine)	484.5	9∗A10 + 3∗A12 + 3∗A14 + 3∗A15 + 3∗A2 + A32 + 2∗A18∗B18 + 4∗A19 + A125 + A121 + 2∗A118 + A119 + A30∗E30	45.43	0	93.77	108.8	45.43	52.7	[31]
$C_{22}H_{21}F$ (2-benzyl-2-fluoro-1, 3-diphenylpropane)	363.6	15∗A10 + 3∗A11 + 2∗A2 + A27 + A4∗B4	24.35	0	66.97	86.1	24.35	31.3	[95]
$C_{22}H_{22}$ (1,1,1-triphenylbutane)	351.1	15∗A10 + 3∗A11 + A1 + A4 + 2∗A2	21.84	0	62.20	79.2	21.84	27.8	[40]
$C_{22}H_{25}NO$ ((±) 5,7,8,15-tetrahydro-3, 4-dimethoxy-6,15-dimethyl-3-benzodioxolo[5,6e][2]benzazecin-14(6)-one (carycavidine))	468.3	Group values unavailable	38.07	0	81.29		38.08		[146]
$C_{22}H_{26}FNO_2$ (1-(4-fluorophenyl)-4-[4-hydroxy-4-(4-methylphenyl)-1-piperidinyl]-1-butanone (moperone))									
Form I	398.2	A14 + 3∗A15 + A17 + A119 + A30∗D30 + A35 + A1 + A24 + 8∗A10 + 2∗A11 + 2∗A12 + 3∗A2	37.4	0	93.9	98.0	37.4	39.0	[205]
Form III	368.2		15.0	0	40.7	98.0	15.0	39.0	
$C_{22}H_{28}N_2O$ (*N*-phenyl-*N*[1-(2-phenylethyl)-4-piperidinyl]-propanamide (fentanyl))	357.2	A14 + 3∗A15 + A16 + A119 + 3∗A2 + 10∗A10 + A11 + A12 + A1 + A59	22.51	0	63.02	95.1	22.51	34.0	[190]

$C_{22}H_{33}NO_3$ (2,2,3,3-tetramethylcyclopropane carboxylic acid cyano(3-phenoxyphenyl) methyl ester (fenpropathrin))	322.5	4∗A1 + A14 + 2∗A17 + A16 + 9∗A10 + A11 + 2∗A12 + A32 + A38 + A56 + A3∗B3	18.57	0	57.58	82.2	18.57	26.5	[155]
$C_{22}H_{42}O_2$ (*cis*-13-docosenoic acid (eurcic acid))	282.2	A1 + 18∗A2∗B2 + 2∗A6 + A36	8.9	31.54					[217]
	307.2		54.0	175.8	207.4	209.0	62.9	64.2	
$C_{22}H_{44}O_2$ (ethyl eicosanoate)	315.0	2∗A1 + A38 + 18∗A2∗B2 + A2	68.62	0	217.8	217.4	68.62	68.5	[92]
$C_{22}H_{44}O_2$ (decyl dodecanoate)	293.2	2∗A1 + A38 + 19∗A2∗B2	63.67	0	217.2	219.7	63.67	64.4	[119]
$C_{22}H_{44}O_2$ (hexyl hexadecanoate)	287.6	2∗A1 + A38 + 19∗A2∗B2	56.19	0	195.4	219.6	56.19	63.2	[119]
$C_{22}H_{46}O_2$ (1,22-docosanediol)	369.7	2∗A30∗B30 + 22∗A2∗B2	39.80	107.7					[15]
	379.4		46.50	122.6	230.3	239.9	86.30	91.0	
$C_{22}H_{46}O_5S_2$ (L-rhamnose dioctyl dithioacetal)	387.9	2∗A1 + 15∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30 (not used in generating the statistics)	54.7	0	141.0	208.1	54.7	80.7	[218]
$C_{23}H_{15}F_{17}OS$ (2-(perfluoro-*n*-octyl)ethylthiomethyl biphenyl-4-yl ether)	362.1	9∗A10 + 3∗A12 + A84 + 3∗A2 + 3∗A25 + 14∗A26∗C26 + 8∗A4∗B4 + A32	47.4	0	130.9	124.3	47.4	45.0	[16]
$C_{23}H_{15}F_{17}S$ (2-(perfluoro-*n*-octyl)-ethylthiomethyl biphenyl-4-yl)	353.2	9∗A10 + 2∗A12 + A11 + A84 + 3∗A2 + 3∗A25 + 14∗A26∗C26 + 8∗A4∗B4	58.3	0	165.1	117.4	58.3	41.5	[16]
$C_{23}H_{26}O_6$ (1,1,1-tris(ethoxycarbonyl)-2,2-diphenylethane)	333.2	3∗A1 + 3∗A2 + 10∗A10 + 2∗A11 + A3 + A4 + 3∗A38	29.5	0	88.54	112.6	29.5	37.5	[85]
$C_{23}H_{28}ClN_3O_5S$ (*N*-[4-(β-(2-methoxy-5-chlorobenzamido)ethyl)-benzosulfonyl]-*N*′-cyclohexylurea (glibenclamide))	450.2	Group values unavailable	53.35	0	118.5		53.35		[183]
$C_{23}H_{36}N_2O_2$ (*N*-(1,1-dimethylethyl)-3-oxo-4-aza-5α-androst-1-ene-17β-carboxamide (finasteride))									
Form I	503.2	4∗A14 + 5∗A15 + 5∗A1 + 2∗A17 + 5∗A16 + A124 + A18∗B18 + B18 + A60 + A4∗B4	4.1	8.1					[202]
	530.2		33.2	62.5	70.6	77.5	37.3	41.1	
Form II	530.2		32.8	0	61.8	77.5	32.8	41.1	
$C_{23}H_{37}BrN_2O_4$ ((4-nitrophenyl)-16-bromohexadecyl carbamate)	382.9	16∗A2∗B2 + A69 + 4∗A10 + 2∗A12 + A50 + A21	62.62	0	163.5	206.3	62.62	79.0	[114]
$C_{23}H_{39}N_3O_3$ (1-hexadecyl-3-(4-nitrophenyl) urea)	392.6	A1 + 15∗A2∗B2 + A66 + 4∗A10 + 2∗A12 + A50	53.94	0	137.4	190.9	53.94	74.9	[114]
$C_{24}H_{24}N_2O_4$ (4-(methoxymethyl)-6-(phenylmethoxy)-9*H*-pyrido-[3,4b]indole-3-carboxylic acid 1-methylethyl ester)	424.0	8∗A10 + 2∗A12 + 2∗A11 + 3∗A1 + 2∗A2 + A14 + 2∗A15 + 4∗A19 + A121 + A41 + A3∗B3 + A38 + 2∗A32	38.83	0	91.58	104.0	38.83	44.1	[180]

Table 6 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{23}H_{27}NO_3S$ (4-(7-undecenyloxy)-phenyl-5-cyano-2-thiophenecarboxylate)	346.1	A14 + 2∗A15 + 4∗A10 + 2∗A12 + A5 + A6 + 2∗A18 + 2∗A19 + A131 + A56 + A32 + A38 + 9∗A2	52.72	0	153.2	147.1	52.72	50.9	[228]
$C_{23}H_{30}O_4S$ (4-(7-undecenyloxy)phenyl-5-methoxy-2-thiophenecarboxylate)	334.1	A14 + 2∗A15 + 4∗A10 + 2∗A12 + A5 + A6 + 2∗A18 + 2∗A19 + A131 + A1 + 2∗A32 + A38 + 9∗A2	61.92	0	185.3	151.7	61.92	50.7	[228]
$C_{23}H_{48}O_2$ (1,23-tricosanediol)	366.3	2∗A30∗B30 + 23∗A2∗B2	41.80	114.1					[15]
	380.7		46.50	122.1	236.2	249.2	88.30	94.9	
$C_{24}H_{48}O_2$ (ethyl docosanoate)	321.0	2∗A1 + A38 + 20∗A2∗B2 + A2 (compound is already in data base, however, the new experimental value is much closer to the predicted entropy)	77.82	0	242.4	236.	77.82	75.8	[92]
$C_{24}H_{50}O_2$ (1,24-tetracosanediol)	372.7	2∗A30∗B30 + 24∗A2∗B2	42.70	114.6					[15]
	381.5		51.20	134.2	248.8	258.5	93.90	98.6	
$C_{24}H_{50}O_5S_2$ (L-rhamnose dinonyl dithioacetal)	342.1	2∗A1 + 17∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	24.7	72.2					[218]
	387.4		54.4	140.4	212.6	222.3	79.1	86.1	
$C_{25}H_{20}$ (tetraphenylmethane)	554.2	20∗A10 + 4∗A11 + A4	48.28	0	87.12	74.8	48.28	41.5	[40]
$C_{25}H_{50}$ (*n*-nonadecylcyclohexane)	317	A14 + 3∗A15 + A1 + A16 + 18∗A2∗B2	77.8	0	245.4	214.8	77.8	68.1	[220]
$C_{25}H_{50}O$ (13-pentacosanone)	347.0	2∗A1 + 22∗A2∗B2 + A35	96.17	0	277.1	244.4	96.17	84.8	[186]
$C_{25}H_{50}O_2$ (ethyl tricosanoate)	326.0	2∗A1 + A38 + 21∗A2∗B2 + A2	57.32	0	175.8	245.3	57.32	80.0	[92]
$C_{26}H_{20}$ (tetraphenylethene)	496.1	2∗A7 + 20∗A10 + 4∗A12	37.45	0	75.49	96.6	37.45	47.9	[99]
$C_{26}H_{54}O_5S_2$ (L-rhamnose didecyl dithioacetal)	332.3	2∗A1 + 19∗A2 + 5∗A3∗B3 + 2∗A84 + 5∗A30∗F30	26.1	78.5					[218]
	385.2		53.2	138.1	216.7	236.5	79.3	91.1	
$C_{27}H_{30}N_2$ (2-(hept-1-ynyl)-5(4-*p*-hexylphenylbuta-1,3-diynyl) pyrimidine)	426.0	2∗A1 + 9∗A2 + 6∗A10 + A11 + 3∗A12 + 6∗A9 + 2∗A41	39.00	0	91.5	116.4	39.00	49.6	[24]
$C_{27}H_{42}Cl_2N_2O_6$ (hexadecanoic acid, [*R*-(*R**,*R**)]-2-[(dichloroacetyl)amino]-3-hydroxy-3-(4-nitrophenyl)propyl ester (chloramphenicol palmitate))	368.2	4∗A10 + A12 + A11 + 3∗A3∗B3 + A1 + A50 + 2∗A22∗F22 + A30∗F30 + A38 + A60 + 15∗A2	64.02	0	173.9	188.7	64.02	69.5	[223–225]
$C_{27}H_{48}$ (17-(1,5-dimethylhexyl)-10, 13-dimethyl-hexadecahydro-1*H*-cyclopenta[a]phenanthrene (5α-cholestane))	351.8	4∗A14 + 5∗A15 + 5∗A1 + 3∗A2 + 2∗A3 + 2∗A17 + 5∗A16	25.4	0	72.20	85.9	25.4	30.2	[148]

$C_{30}H_{32}P_2$ (1,6-bis(diphenylphosphino)-hexane)	399.4	2∗A72 + 20∗A10 + 4∗A12 + 6∗A2	66.8	0	167.2	119.2	66.8	47.6	[128]
$C_{30}H_{40}N_4O_2$ (α,ω-bis(azobenzene-4-oxy)hexane)	442.2	18∗A10 + 6∗A12 + 6∗A2 + 4∗A42 + 2∗A32	73.53	0	166.3	133.0	73.53	58.8	[143]
$C_{31}H_{32}O_2P_2$ ((−) 2,3-*O*-isopropylidene-2,3-dihydroxy-1,4-bis(diphenylphosphino)butane)	348.7	A14 + 2∗A15 + 2∗A112 + 2∗A1 + 2∗A16 + A17 + 2∗A2 + 20∗A10 + 4∗A12 + 2∗A72	3.42	9.81					[112]
	364.2		38.61	106.0	115.8	105.2	42.03	38.3	
$C_{36}H_{30}Si_3O_3$ (hexaphenylcyclotrisiloxane)	455	30∗A10 + 6∗A11 + A14 + 3∗A15 + 3∗A112 + 3∗A139	1.13	2.48					[221]
	466		39.3	84.33	86.8	108.4	40.43	50.51	
$C_{38}H_{68}N_2O_2$ (*N*,*N*′-dihexadecanoylbenzene-1,2-diamine)	367.2	4∗A10 + 2∗A12 + 2∗A1 + 2∗A60 + 28∗A2∗B2	78.0	212.4					[227]
	388.2		32.0	82.43	294.8	313.2	110.0	121.6	
$C_{39}H_{78}O$ (20-nonatricontanone)	365.8	38∗A2∗B2 + A35 + 2∗A1	153.0	0	418.5	374.6	153.0	137.0	[186]
$C_{41}H_{84}$ (hentetracontane)	357.5	2∗A1 + 39∗A2∗B2	147.2	0	402.4	397.4	147.2	138.8	[151]
$C_{48}H_{40}P_2$ (2,2′-bis(di-4-toluenephosphino)-1,1′-binaphthyl)	528.3	4∗A1 + 28∗A10 + 4∗A11 + 12∗A12 + 2∗A72	41.98	0	79.46	107.8	41.98	57.0	[118]
$C_{48}H_{40}SI_4O_4$ (octaphenylcyclotetrasiloxane)	348	40∗A10 + 8∗A11 + A14 + 5∗A15 + 4∗A112 + 4∗A139	2.22	6.38					[221]
	463		46.4	100.2					
	475		1.13	2.38	109.0	137.1	49.78	65.1	
$C_{51}H_{104}$ (*n*-henpentacontane)	337	2∗A2 + 49∗A2∗B2	1.75	5.2					[241]
	343		5.3	15.5					
	365.6		170.4	466.1	486.8	469.9	177.5	171.8	
$C_{52}H_{106}$ (*n*-dopentacontane)	352	2∗A2 + 50∗A2∗B2	17.1	48.6					[241]
	366.7		171.8	468.5	517.1	500.3	188.9	183.4	
$C_{60}F_{48}$ (fluorinated fullerene)	329.6	Enthalpy of fusion not determined	7.0	21.24					[56]
$C_{192}H_{386}$ (*n*-dononacontahectane)	399.1	2∗A1 + 190∗A2∗B2 (not used in generating the statistics)	661.1	0	1656.5	1802	661.1	719.3	[233]

[a] Corrected to 298 K.

[b] Experimental enthalpies of fusion and melting point temperatures were obtained through correspondence with the authors.

[c] Authors report only an entropy of transition and a temperature range for the first two transitions. The temperature that is listed is the midpoint of the reported temperature range and the transition enthalpy is computed as the product of the reported transition entropy times transition temperature as defined above.

[d] Compound used was only 83% crystalline. Authors reported a corrected value of 7.77 kJ mol^{-1} for the enthalpy of fusion for a sample of 100% degree of crystallinity.

[e] Experimental fusion enthalpy (in J g^{-1}) was taken from graph.

above. Examples can be found in Table 6. Molecules that contain both benzenoid and cyclic carbon atoms, such as fluorene require some additional comments. In such cases, the ring Eq. (2) is used to model the non-benzenoid ring. Any quaternary benzenoid carbon atoms that constitute part of a non-benzenoid ring are treated as cyclic quaternary sp^2 carbon atoms. Thus, the five-member ring in fluorene is modeled as a tetrasubstituted cyclopentadiene ring. The remaining eight tertiary benzenoid carbon atoms making up the remainder of the aromatic ring are added as additional substituents once the contribution of the tetrasubstituted cyclopentadiene ring is computed. Additional examples can be found in Table 6.

2.3.2. Cyclic functional groups

Estimations of molecules containing functional groups that form part of a non-benzenoid ring are computed in a similar manner. The ring Eq. (2) or (3) is first used to model a hydrocarbon ring of similar size and structure. The functional groups that comprise a portion of the ring are added as adjustments to the calculation. Group values for cyclic functional groups can be found in Table 5. The single group coefficient found in Table 4 for a cyclic tertiary sp^2 carbon is used to compute the contribution of this group whenever a cyclic functional group is directly attached to this type of carbon.

2.3.3. Evaluation of new group values

New group values have been assigned by allowing the new group value to vary until the value of the following function.

$$\sum \left[\frac{\Delta_0^{T_{fus}} S_{tpce}(\text{exp}) - \Delta_0^{T_{fus}} S_{tpce}(\text{calcd})}{\Delta_0^{T_{fus}} S_{tpce}(\text{exp})} \right]^2$$

was minimized. All the compounds used in generating these new group values are included in Tables 6–8 and are identified by the alphanumeric values A147–A161. Not all the compounds used in changing existing group values are included in these tables. Fusion enthalpies for some of the compounds have been reported in a previous publication [2].

3. Estimation of total phase change enthalpy

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

4. Total phase change entropies of non-isotropic systems

As noted earlier, the group values listed in Tables 1–5 generally overestimate the total phase change entropy

Table 7
Polymers

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
C_5H_8 (poly(3-methyl-1-butene))	584	2∗A1 + A2 + A3	6.04	0	10.3	9.5	6.04	5.5	[20]
$C_5H_{12}Si$ (poly[sil(dimethyl)-trimethylene])	325	2∗A1 + 3∗A2∗B2 + A109	8.49	0	26.1	36.0	8.49	11.7	[211]

Narrative continues on pg. 106.

Table 8
Molar transition enthalpies (kJ mol^{-1}) and entropies (J mol^{-1} K^{-1}) of select amphiphilic semiperfluorinated–semiperhydrogenated di- and triblock organic compounds[a]

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
Unsubstituted diblock molecules									
$C_{14}H_5F_{25}$ ($F_3C(CF_2)_{11}(CH_2)_2H$)	344.0	3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + A2 + A1 (no solid–solid transitions observed above room temperature)	20.4	0	60.5	79.4	20.4	16.7	[196]
$C_{16}H_9F_{25}$ ($F_3C(CF_2)_{11}(CH_2)_4H$)	147.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 3∗A2 + A1)	0.7	5					[192,196]
	314.0		1.4	4					
	349.0		21.0	61	69.4	57.1 (93.6)	23.1	19.9	
$C_{16}H_{13}F_{21}$ ($F_3C(CF_2)_9(CH_2)_6H$)	306.0	0.61∗(3∗A25 + 18∗A26∗B26 + 10∗A4∗B4 + 5∗A2 + A1)	4.2	14					[192]
	318.0		16.9	53	67	61.6 (100.9)	21.1	19.6	
$C_{16}H_{17}F_{17}$ ($F_3C(CF_2)_7(CH_2)_8H$)	301.2	0.61∗(7∗A2 + A1 + 8∗A4∗B4 + 3∗A25 + 17∗A26∗B26)	9.5	31.6					[208]
	303.2		5.7	18.8	50.3	90.2 (147.9)	15.2	27.3	
$C_{17}H_{21}F_{15}$ ($(CF_3)_2CF(CF_2)_4(CH_2)_{10}H$)	220.0	0.61∗(6∗A25 + 8∗A26∗B26 + A27 + 7∗A4∗B4 + 9∗A2∗B2 + A1)	3	13.6					
	261.0		18	69.0	82.6	84.6 (138.6)	21	18.9	[194]
$C_{18}H_{13}F_{25}$ ($F_3C(CF_2)_{11}(CH_2)_6H$)	164.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 5∗A2 + A1)	0.5	1					[192,196]
	316.0		3.5	11					
	357.0		23.4	65.5	79.7	65.7 (107.8)	27.4	23.5	
$C_{18}H_{21}F_{17}$ ($F_3C(CF_2)_7(CH_2)_{10}H$)	288.0	0.61∗(3∗A25 + 14∗A26∗B26 + 8∗A4∗B4 + 9∗A2∗B2 + A1)	3.5	12					[192]
	308.0		20.2	65	77.7	86.8 (142.3)	23.7	26.9	
$C_{19}H_{21}F_{19}$ ($(CF_3)_2CF(CF_2)_6(CH_2)_{10}H$)	274.0	0.61∗(6∗A25 + 12∗A26∗B26 + A27 + 9∗A4∗B4 + 9∗A2∗B2 + A1)	1	3.6					[194]
	298.0		25	83.9	87.5	84.6 (138.6)	26	22.1	
$C_{20}H_{17}F_{25}$ ($F_3C(CF_2)_{11}(CH_2)_8H$)	192.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 7∗A2 + A1)	2.4	12.5					[192,196]
	329.0		6.4	19.5					
	361.0		23.7	65.7	97.6	74.7 (122)	32.5	26.9	
$C_{20}H_{21}F_{21}$ ($F_3C(CF_2)_9(CH_2)_{10}H$)	317.0	0.61∗(3∗A25 + 18∗A26∗B26 + 10∗A4∗B4 + 9∗A2 + A1)	4.0	12					[192]
	337.0		24.4	72	85	78.9 (129.3)	28.4	26.6	
	310.5		2.2	7.1					
	336.7		26.7	79.3	86.4	78.9 (129.3)	28.9	26.6	[208]
$C_{21}H_{25}F_{19}$ ($(CF_3)_2CF(CF_2)_6(CH_2)_{12}H$)	310.0	0.61∗(6∗A25 + 12∗A26∗B26 + A27 + 9∗A4∗B4 + 11∗A2∗B2 + A1)	34	0	109.7	100.1 (164.1)	34	31.0	[194]

Table 8 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{22}H_{21}F_{25}$ ($F_3C(CF_2)_{11}(CH_2)_{10}H$)	207.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 9∗A2 + A1)	1.0	6					[192,196]
	342.0		9.5	28					
	365.0		25.8	71	103.3	83.1 (136.2)	36.3	30.3	
$C_{22}H_{25}F_{21}$ ($F_3C(CF_2)_9(CH_2)_{12}H$)	334.0	0.61∗(3∗A25 + 18∗A26∗B26 + 10∗A4∗B4 + 11∗A2∗B2 + A1)	6	19					[194]
	338.0		27	79.9	97.8	102.3 (167.7)	33	34.6	
$C_{24}H_{25}F_{25}$ ($F_3C(CF_2)_{11}(CH_2)_{12}H$)	216.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 11∗A2 + A1)	1.8	8					[196]
	352.0		10.2	30					
	364.0		25.8	70.9	108.2	91.7 (150.4)	37.8	33.4	
$C_{24}H_{25}F_{25}$ ($F_3C(CF_2)_{11}CH_2$-$CH(CH_3)(CH_2)_9H$)	260.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 10∗A2 + 2∗A1 + A3)	9	34.6					[194]
	347.0		25	72.0	106.7	88.1 (144.5)	34	30.6	
$C_{26}H_{29}F_{25}$ ($F_3C(CF_2)_{11}(CH_2)_{14}H$)	363.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 13∗A2∗B2 + A1)	16.3	45					[192,193,196]
	366.0		26.1	73	116.2	117.9 (193.2)	42.4	43.1	
$C_{28}H_{33}F_{25}$ ($F_3C(CF_2)_{11}(CH_2)_{16}H$)	367.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 15∗A2∗B2 + A1)	41.8	0	113.9	129.2 (211.8)	41.8	47.4	[196]
$C_{30}H_{37}F_{25}$ ($F_3C(CF_2)_{11}(CH_2)_{18}H$)	370.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 17∗A2∗B2 + A1)	49.7	0	134.3	140.5 (230.4)	49.7	52.0	[196]
$C_{32}H_{41}F_{25}$ ($F_3C(CF_2)_{11}(CH_2)_{20}H$)	250.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 19∗A2∗B2 + A1) (independent measurement on compound; no solid phase transitions reported)	4.1	16.4					[196,197]
	308.0		7.9	25.6					
	373.0		58.0	155.5	197.5	151.9 (249)	70	56.7	
	369.2		43.4	0	117.6	135.9	43.4	56.1	
Unsubstituted triblock molecules									
$C_{28}H_{16}F_{42}$ ($F_3C(CF_2)_9(CH_2)_8(CF_2)_9CF_3$)	272.2	0.61∗(6∗A25 + 36∗A26∗B26 + 20∗A4∗B4 + 8∗A2)	9.2	34					[196]
	387.0		57.1	149	181.3	93.0 (152.4)	66.3	36.0	
$C_{34}H_{20}F_{50}$ ($F_3C(CF_2)_{11}(CH_2)_{10}$-$(CF_2)_{11}CF_3$)	297.0	0.61∗(10∗A2 + 24∗A4∗B4 + 44∗A26∗B26 + 6∗A25)	3.3	11.1					[195]
	371.0		3.5	9.4					
	402.0		55.1	137.1	157.6	110.0 (180.4)	61.9	32.6	
Brominated diblock molecules									
$C_{10}H_4BrF_{17}$ ($F_3C(CF_2)_7(CH_2)_2Br$)	297.8	0.61∗(3∗A25 + 14∗A26∗B26 + 8∗A4∗B4 + 2∗A2 + A21)	13.9	0	46.7	51.1 (83.7)	13.9	15.2	[191]

$C_{12}H_8BrF_{17}$ ($F_3C(CF_2)_7(CH_2)_4Br$)	308.0	0.61*(3*A25 + 14*A26*B26 + 8*A4*B4 + 4*A2 + A21)	20.8	0	67.5	59.7 (97.9)	20.8	18.4	[191]
$C_{14}H_{12}BrF_{17}$ ($F_3C(CF_2)_7(CH_2)_6Br$)	311.7	0.61*(3*A25 + 14*A26*B26 + 8*A4*B4 + 6*A2 + A21)	27.6	0	88.5	68.4 (112.1)	27.6	21.3	[191]
$C_{18}H_{20}BrF_{17}$ ($F_3C(CF_2)_7$-$(CH_2)_{10}Br$)	317.2	0.61*(3*A25 + 14*A26*B26 + 8*A4*B4 + 10*A2*B2 + A21)	38.5	0	121.4	99.2 (162.6)	38.5	31.5	[191]
$C_{20}H_{20}BrF_{21}$ ($F_3C(CF_2)_9$-$(CH_2)_{10}Br$)	343.9	0.61*(3*A25 + 18*A26*B26 + 10*A4*B4 + 10*A2 + A21)	32.3	0	93.9	91.9 (150.6)	32.3	31.6	[191]
Diblock alcohol molecules									
$C_{14}H_9F_{21}O$ ($F_3C(CF_2)_9$-$(CH_2)_4OH$)	360.0	0.61*(3*A25 + 18*A26*B26 + 10*A4*B4 + 4*A2 + A30*B30)	21.3	0	59	66.0 (108.1)	21.3	23.7	[192]
$C_{16}H_9F_{25}O$ ($F_3C(CF_2)_{11}$-$(CH_2)_4OH$)	374.0	0.61*(3*A25 + 22*A26*B26 + 12*A4*B4 + 4*A2 + A30*B30)	1.4	3.7					[192]
	394.0		26.3	67	70.5	72.1 (118.2)	27.7	28.4	
$C_{16}H_{13}F_{21}O$ ($F_3C(CF_2)_9$-$(CH_2)_6OH$)	364.0	0.61*(3*A25 + 18*A26*B26 + 10*A4*B4 + 6*A2 + A30*B30)	25.4	0	69.8	74.6 (122.3)	25.4	27.2	[192]
$C_{16}H_{17}F_{17}O$ ($F_3C(CF_2)_7$-$(CH_2)_8OH$)	231.0		1.2	5.2					
	333.0	0.61*(3*A25 + 14*A26*B26 + 8*A4*B4 + 8*A2 + A30*B30)	19.2	57.7	62.9	77.2 (126.5)	20.4	25.7	[192]
$C_{16}H_{19}F_{15}O$ ($F_3C(CF_2)_6CH(OH)(CH_2)_8H$)	325.0	0.61*(3*A25 + 12*A26*B26 + 7*A4*B4 + 7*A2 + A1 + A3*B3 + A30*B30)	3.9	12					[195]
	332.5		23.2	69.8	81.8	74.5 (122.1)	27.1	24.8	
$C_{18}H_{13}F_{25}O$ ($F_3C(CF_2)_{11}$-$(CH_2)_6OH$)	392.0	0.61*(3*A25 + 22*A26*B26 + 12*A4*B4 + 6*A2 + A30*B30)	29.5	0	75.3	80.7 (132.4)	29.5	31.6	[192]
$C_{18}H_{17}F_{17}O$ ($F_3C(CF_2)_7$-$(CH_2)_{10}OH$)	351.0	0.61*(3*A25 + 14*A26*B26 + 8*A4*B4 + 10*A2*B2 + A30*B30)	29.4	0	83.8	99.3 (162.7)	29.4	34.8	[192]
$C_{20}H_{21}F_{21}O$ ($F_3C(CF_2)_9$-$(CH_2)_{10}OH$)	265.0	0.61*(3*A25 + 18*A26*B26 + 10*A4*B4 + 10*A2 + A30*B30)	3.4	12.8					[192]
	376.0		35.1	93.4	106.2	91.9 (150.7)	38.5	34.8	
$C_{20}H_{23}F_{19}O$ ($F_3C(CF_2)_8CH(OH)(CH_2)_{10}H$)	346.2	0.61*(3*A25 + 16*A26*B26 + 9*A4*B4 + 9*A2 + A1 + A3*B3 + A30*B30)	3.6	10.4					[195]
	356.0		33.5	94.1	104.5	89.3 (146.4)	94.4	31.7	
$C_{22}H_{21}F_{25}O$ ($F_3C(CF_2)_{11}(CH_2)_{10}OH$)	396.0	0.61*(3*A25 + 22*A26*B26 + 12*A4*B4 + 10*A2 + A30*B30)	40.0	0	101	98.1 (160.8)	40.0	38.8	[192]
Diblock allyl ether molecules									
$C_{16}H_{17}F_{17}O$ ($F_3C(CF_2)_7$-$(CH_2)_6OCH_2CH{=}CH_2$)	238.0	0.61*(3*A25 + 14*A26*B26 + 8*A4*B4 + 7*A2 + A32 + A6 + A5)	0.8	3.3					[192]
	276.0		4.4	15.9					
	283.0		13.0	45.9	65.2	78.7 (129.1)	18.2	22.3	

Table 8 (*Continued*)

Compound	T (K)	Calculation	ΔH_{pce}	ΔS_{pce}	ΔS_{tpce}		ΔH_{tpce}		Reference
					Experimental	Calculated	Experimental	Calculated	
$C_{17}H_{13}F_{21}O$ ($F_3C(CF_2)_9$-$(CH_2)_4OCH_2CH{=}CH_2$)	217.0	0.61∗(3∗A25 + 18∗A26∗B26 + 10∗A4∗B4 + 5∗A2 + A32 + A6 + A5)	1.9	8.8					[192]
	286.0		4.4	15.4					
	309.0		13.9	45.0	69.1	76.2 (124.9)	20.2	23.5	
$C_{17}H_{17}F_{17}O$ ($F_3C(CF_2)_7$-$(CH_2)_6OCH_2CH{=}CH_2$)	238.0	0.61∗(8∗A4∗B4 + 14∗A26∗B26 + A5 + A6 + 7∗A2 + A32 + 3∗A25)	0.8	3.4					[192]
	276.0		4.4	15.9					
	283.1		13.0	45.9	65.2	78.7 (129.1)	18.2	22.3	
$C_{19}H_{13}F_{25}O$ ($F_3C(CF_2)_{11}$-$(CH_2)_4OCH_2CH{=}CH_2$)	208.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 5∗A2 + A32 + A6 + A5)	1.3	6.3					[192]
	291.0		3.9	13.4					
	355.0		21.5	60.6	80.2	82.3 (134.9)	26.7	29.2	
$C_{19}H_{17}F_{21}O$ ($F_3C(CF_2)_9$-$(CH_2)_6OCH_2CH{=}CH_2$)	222.0	0.69∗(3∗A25 + 18∗A26∗B26 + 10∗A4∗B4 + 7∗A2 + A32 + A6 + A5)	1.4	6.3					[192]
	306.0		4.6	15.0					
	322.0		17.3	53.7	75.1	84.8 (139.1)	23.3	27.3	
$C_{21}H_{17}F_{25}O$ ($F_3C(CF_2)_{11}$-$(CH_2)_6OCH_2CH{=}CH_2$)	215.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 7∗A2 + A32 + A6 + A5)	3.1	14.4					[192]
	320.0		6.8	21.3					
	360.0		22.3	61.9	97.6	91.0 (149.1)	32.2	32.7	
$C_{21}H_{25}F_{17}O$ ($F_3C(CF_2)_7$-$(CH_2)_{10}OCH_2CH{=}CH_2$)	263.0	0.61∗(3∗A25 + 14∗A26∗B26 + 8∗A4∗B4 + 11∗A2 + A32 + A6 + A5)	3.0	11.4					[192]
	301.0		26.5	88	99.4	96 (157.5)	29.5	28.9	
$C_{23}H_{27}F_{21}O$ ($F_3C(CF_2)_9$-$(CH_2)_{10}OCH_2CH{=}CH_2$)	253.0	0.61∗(3∗A25 + 18∗A26∗B26 + 10∗A4∗B4 + 11∗A2 + A32 + A6 + A5)	2.1	8.3					[192]
	333.0		32.9	98.7	107.1	102.2 (167.5)	35.0	34.0	
$C_{25}H_{25}F_{25}O$ ($F_3C(CF_2)_{11}$-$(CH_2)_{10}OCH_2CH{=}CH_2$)	250.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 11∗A2 + A32 + A6 + A5)	2.0	8					[192]
	348.0		13.9	39.9					
	364.0		23.7	65.1	113.1	108.3 (177.5)	39.6	39.4	
Diblock ester molecules									
$C_{13}H_7F_{17}O_2$ ($F_3C(CF_2)_7$-$(CH_2)_2OOCCH{=}CH_2$)	253.2	0.61∗(3∗A25 + 14∗A26∗B26 + 7∗A4∗B4 + 2∗A2 + A38 + A6∗B6 + A7)	6.9	27.3					[229]
	268.2		6.6	24.6	51.9	55.0 (90.2)	13.5	14.8	

$C_{14}H_9F_{17}O_2$ ($F_3C(CF_2)_7$-$(CH_2)_2OOCC(CH_3)=CH_2$)	210.0	0.61∗(3∗A25 + 14∗A26∗B26 + 10∗A4∗B4 + 2∗A2 + A1 + A38 + A5 + A7)	5	23.8					[193]
	253.0		9	35.6	59.3	59.9 (98.1)	14.0	15.1	
$C_{18}H_{13}F_{21}O_2$ ($F_3C(CF_2)_9$ $(CH_2)_4OOCC(CH_3)=CH_2$)	297.0	0.61∗(3∗A25 + 18∗A26∗B26 + 10∗A4∗B4 + 4∗A2 + A1 + A38 + A5 + A7)	10	33.7					[193]
	311.0		0.5	1.6					
	319.0		15	47.0	82.3	74.6 (122.4)	25.5	23.8	
$C_{20}H_{13}F_{25}O_2$ ($F_3C(CF_2)_{11}$-$(CH_2)_4OOCC(CH_3)=CH_2$)	297.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 4∗A2 + A1 + A38 + A5 + A7)	10	33.7					[193]
	301.0		0.4	1.3					
	360.0		21	58.3	93.3	80.8 (132.4)	31.4	29.1	
$C_{20}H_{17}F_{21}O_2$ ($F_3C(CF_2)_9$-$(CH_2)_6OOCC(CH_3)=CH_2$)	306.0	0.61∗(3∗A25 + 18∗A26∗B26 + 10∗A4∗B4 + 6∗A2 + A1 + A38 + A5 + A7)	14	45.8					[193]
	311.0		1	3.2					
	321.0		15	46.7	95.6	83.3 (136.6)	30	26.7	
$C_{22}H_{17}F_{25}O_2$ ($F_3C(CF_2)_{11}$-$(CH_2)_6OOCC(CH_3)=CH_2$)	312.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 6∗A2 + A1 + A38 + A5 + A7)	12	38.5					[193]
	320.0		1	3.1					
	363.0		22	60.6	102.2	89.4 (146.6)	35	32.5	
$C_{26}H_{25}F_{25}O_2$ ($F_3C(CF_2)_{11}$-$(CH_2)_{10}OOCC(CH_3)=CH_2$)	337.0	0.61∗(3∗A25 + 22∗A26∗B26 + 12∗A4∗B4 + 10∗A2 + A1 + A38 + A5 + A7)	5	14.8					[193]
	368.0		21	57.1	71.9	106.8 (175)	26	39.3	
Miscellaneous diblock molecules									
$C_{16}H_{17}F_{15}O$ ($F_3C(CF_2)_6(C=O)(CH_2)_7CH_3$)	285.8	7∗B4∗A4 + 3∗A25 + 12∗A26∗B26 + A1 + 7∗A2 + A35 (no mesophase formed; normal calculation used)	34.2	0	119.7	118.9	34.2	34.0	[208]
$C_{20}H_{21}F_{19}O$ ($F_3C(CF_2)_8CO(CH_2)_{10}H$)	317.9	(9∗B4∗A4 + 3∗A25 + 16∗A26∗B26 + A1 + 9∗A2 + A35) (no mesophase formed; normal calculation used)	53.1	0	167.1	143.2	53.1	45.5	[208]
$C_{20}H_{20}F_{21}I$ ($F_3C(CF_2)_9CH_2CHI)(CH_2)_8H$)	328.0	0.61∗(3∗A25 + 18∗A26∗B26 + 10∗A4∗B4 + 8∗A2 + A1 + A3∗B3 + A29)	19.2	0	58.5	89.1 (146)	19.2	29.2	[208]
$C_{22}H_{29}F_{17}S$ ($F_3C(CF_2)_7(CH_2)S(CH_2)_{12}H$)	276.0	0.61∗(3∗A25 + 14∗A26∗B26 + 8∗A4∗B4 + 13∗A2∗B2 + A1 + A84)	2.9	10.5					[192]
	310.0		29.1	93.9	104.4	113.3 (185.7)	32.0	37.2	

[a] The value in parenthesis corresponds to the total phase change entropy evaluated at a fraction of 1.

of molecules that do not behave isotropically in the liquid state. This results in total phase change enthalpies that are considerably larger than what is observed experimentally. In liquid crystals, even if all the transition entropies are added together, their sum is usually considerably less that what is estimated by these group values, usually by a substantial amount. There may be several reasons for this. Once the solid has melted all entropy increases associated with increases in translational and rotational freedom in the mesophase may not occur isothermally. Some of the entropy change associated with the phase change may be incorporated into the heat capacity changes occurring during the mesophase. Another possibility is that these systems may not become completely isotropic in the liquid except at temperatures well above the mesophase to isotropic liquid phase transition. The presence of additional undetected transitions occurring below room temperature is also a possibility. The estimation of the partially fluorinated diblock hydrocarbons, summarized in Table 8, illustrate this point quite clearly. The total phase change entropy of these compounds can be obtained by noting that the experimental value measured amounts to a relatively constant fraction of the total phase change entropy expected of a totally isotropic molecule of this structure. This fraction amounts to 0.61 of the total phase change entropy expected. Some partially fluorinated molecules that apparently do not form a mesophase appear to be estimated in the normal fashion (e.g. see $C_{16}H_{17}F_{15}O$ and $C_{20}H_{21}F_{19}O$ in Table 8) while others are not (e.g. see $C_{21}H_{25}F_{19}$, $C_{28}H_{33}F_{25}$ and $C_{30}H_{37}F_{25}$ in Table 8). Diblock molecules have been estimated in the normal fashion. Fluorine substitution is considered a single substituent regardless of the number attached. The group coefficient for a methylene group has been used in cases where the number of consecutive CH_2, equals or exceed the sum of the other remaining carbon atoms and other functional groups. Examples are found in Table 8.

Thermal data for very few triblock molecules are available. It is difficult to reach any conclusions regarding this class of partially fluorinated compounds.

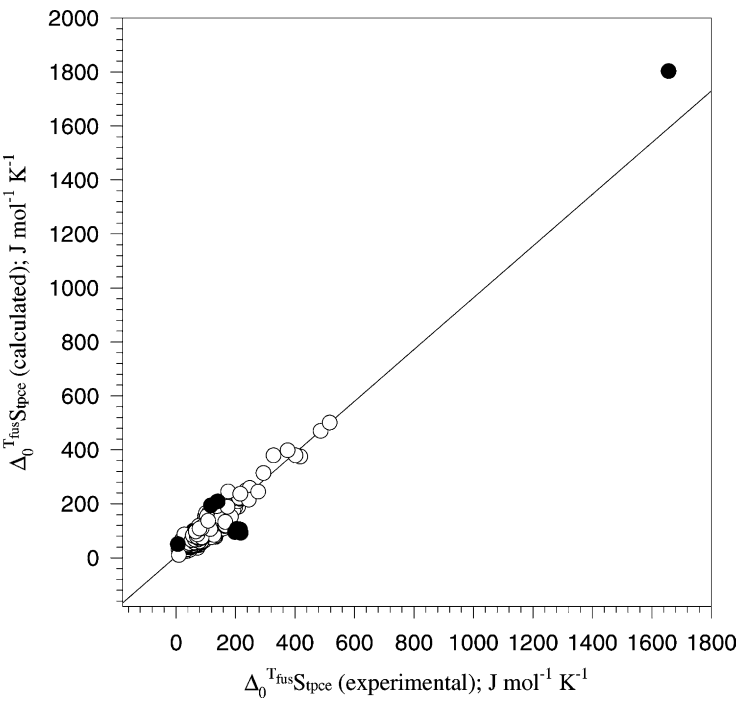

Fig. 1. A comparison of calculated and experimental total phase change entropies. The solid circles represent data that exceeded three standard deviations and were not used in generating the statistics or the equation of the line through the data.

5. Statistics of the correlations

Excluding the non-isotropic molecules, fusion enthalpies and entropies of a total of 556 compounds are included in this compendium. Most measurements are on new compounds. A few measurements are new measurement on compounds reported in earlier versions of this work. A total of nine compounds had errors greater than three standard deviations. The values of these compounds are not included in generating the statistics given below but are included in the graphical presentation of the correlations given in Figs. 1 and 2. Fig. 1 illustrates the correlation obtained when experimental total phase change entropies are compared to those estimated using the protocol described above for compounds melting directly to an isotropic liquid. The standard deviation between experiment and calculation is ± 18.6 J mol^{-1} K^{-1} for 547 compounds. Many of the compounds correlated are structurally complex. Eighteen new groups have been added to Tables 2 and 3 and values for 11 groups reported previously have been changed as a consequence of the additional data. If the compounds used to establish new group values and revise existing group values are removed from the database, the standard deviation between experiment and calculation of the remaining 463 compounds changes to ± 19.1 J mol^{-1} K^{-1}. This compares to a standard deviation of ± 18.4 J mol^{-1} K^{-1} obtained previously for 260 test compounds [1]. The average fractional error was approximately 0.25 for both total phase change entropy and enthalpy. If nine compounds with

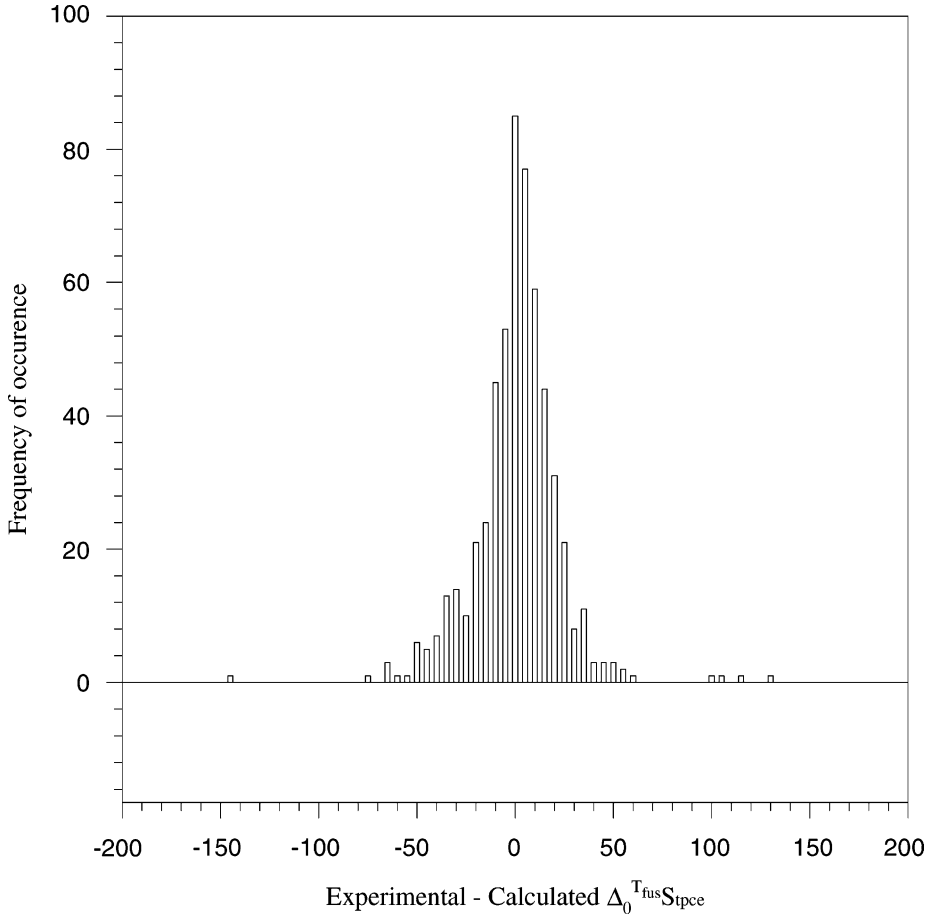

Fig. 2. A histograph illustrating the distribution of errors in $\Delta_0^{T_{fus}}S_{tpce}$.

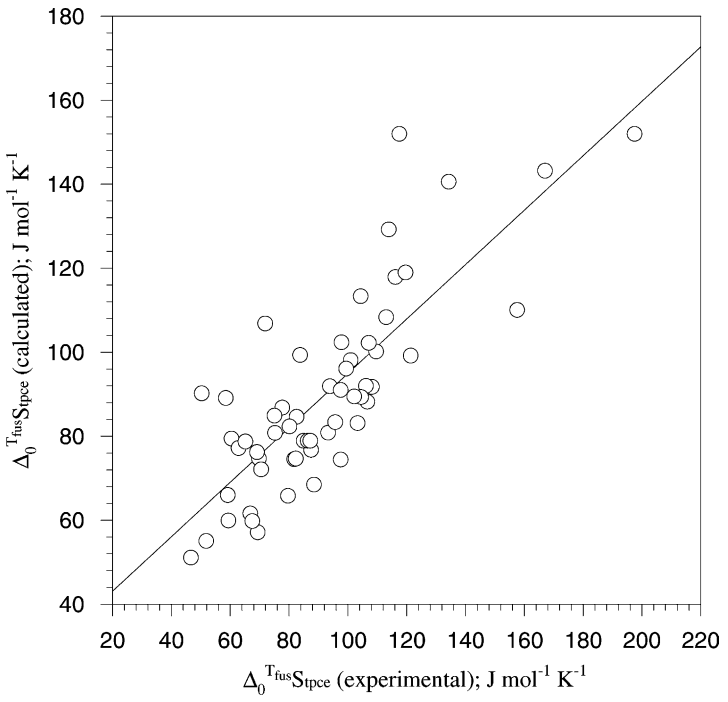

Fig. 3. A comparison of calculated and experimental total phase change entropies for the partially fluorinated amphiphilic compounds.

fractional errors greater than one are excluded from the data base, fractional errors of 0.192 and 0.198 are obtained for total phase change entropy and enthalpy, respectively. These results are in line with the fractional errors obtained previously (0.181 and 0.194, respectively). In many of the compounds with significant errors, the experimental $\Delta_0^{T_{fus}}S_{tpce}$ is considerably smaller that the value estimated, strongly suggesting the presence of additional but yet undetected phase changes.

The equation of the line obtained by a linear regression of the data in Fig. 1 is given by:

$$\Delta_0^{T_{fus}}S_{tpce}(\text{calcd}) = (0.958 \pm 0.014)\Delta_0^{T_{fus}}S_{tpce}(\text{exp}) + (5.3 \pm 18.6); \quad r^2 = 0.8926 \tag{5}$$

The scatter associated with this correlation as indicated by the correlation coefficient is similar to that obtained previously for 1858 compounds (0.8962). Compounds indicated by the solid circles were characterized by errors greater than three standard deviations and were not used in generating Eq. (5). The distribution of errors for the 556 compounds is shown in Fig. 2.

Correlation of the total phase change entropies of the partially fluorinated molecules is shown in Fig. 3. The equation of the line obtained by a linear regression analysis is given by:

$$\Delta_0^{T_{fus}}S_{tpce}(\text{calcd}) = (0.648 \pm 0.06)\Delta_0^{T_{fus}}S_{tpce}(\text{exp}) + (30.1 \pm 13.5); \quad r^2 = 0.6525 \tag{6}$$

A total of 58 compound were correlated resulting in a standard deviation of ± 16.7 J mol^{-1} K^{-1} when the differences between experimental and calculated results are compared.

Total phase change enthalpies were obtained by multiplying the estimated total phase change entropy by the fusion temperature. For the 548 compounds considered in the database, a standard deviation of ± 7.4 kJ mol^{-1} was obtained (excluding those with errors of $\geq |\pm 3\sigma|$. The standard error associated with the 58 diblock molecules was ± 5.5 kJ mol^{-1} with one entry in excess of three standard deviations.

Direct estimation of fusion enthalpies by group additivity has previously been reported by Joback and Reid [3]. These workers report a fractional error in estimated fusion enthalpies of 0.39. The error associated with this group method, however, cannot be directly compared to the results reported here. The estimates associated with the Joback and Reid method refer to direct estimates of fusion enthalpy. The uncertainties reported in this work refer to uncertainties associated with the sum of all enthalpies associated with phase changes occurring from 0 K to the isotropic liquid at the melting point.

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