Critically Evaluated Thermochemical Properties of Polycyclic Aromatic Hydrocarbons

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Experimental thermochemical properties of benzene, toluene, and 63 polycyclic aromatic hydrocarbons, published within the period 1878–2008 (over 350 references), are reported. Available experimental data for the enthalpies of combustion used to calculate enthalpies of formation in the condensed state, combined with sublimation, vaporization, and fusion enthalpies, are critically evaluated. Whenever possible, recommended values for these thermochemical properties and for the enthalpies of formation in the gas state at $T = 298.15$ K are provided. © *2008 American Institute of Physics*.

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1. Introduction

Enthalpies of formation are crucial thermodynamic quantities. They are needed to evaluate the amount of energy released or absorbed in a chemical reaction and to calculate other thermodynamic functions, such as Gibbs energies and equilibrium constants, and more importantly, they permit a quantitative assessment of the relative stability of a molecule. Polycyclic aromatic compounds, both hydrocarbons and heterocycles, are very important ones and have attracted great attention. These materials play an important role in interstellar chemistry [1996COO/SCH, 1995SNO/WIT, 1987LEG/DHE], geochemistry, especially in relation to the origin of petroleum [1999GOL], and environmental chemistry [1997HAR]. They are produced mainly by the incomplete combustion or pyrolysis of organic materials, hydrocarbon fuels, and coal conversion processes and are precursors of soot. They are formed throughout the environment as by-products of combustion and degradation of organic materials in industrial processes. Factors such as the type and quantity of fuel consumed, temperature, time of combustion, and availability of oxygen determine the nature and degree of formation of these materials. Polycyclic aromatic hydrocarbons (PAHs) have relatively low vapor pressure and resistance to chemical reactions. As a result, they are persistent in the environment and show a tendency to accumulate in living beings, soils, and sediments and are also highly dispersed by the atmosphere [1997HAR]. However, control of their emissions is an important matter because of the potential adverse health effects on humans associated with exposure to these substances. In fact, many PAHs are among the well known carcinogenic or mutagenic products [2005LUC].

The prediction of the behavior and reaction kinetics of PAHs requires an accurate description of their thermochemical properties. In addition, thermochemical values, such as their enthalpies of formation, are useful in predicting the likelihood of their formation. These properties are also useful in designing processes to generate other useful substances such as the fullerenes [2006WID/MCC, 1999RIC/GRI] which retain some known PAH substructure [1996TAY, 1993KRO/WAL, 1993KRO/FIS, 1993BIL/CIU] and other carbon nanostructures [2006OKI/OTA, 1996DRE/DRE].

Available experimental thermochemical data on PAHs are scarce mainly due to the difficulty in their synthesis and purification. Moreover, the reliability of the existing results varies because of the different experimental techniques used and the large time frame, 1878–present, in which they have been studied. As their molar masses increase, the number of isomeric PAHs likewise increases significantly. Large molecular mass PAHs have high melting points and low vapor pressures; in addition they become less soluble in organic solvents. Thus, it is often not easy to separate isomers and samples are often contaminated by the presence of certain other isomers. The sublimation enthalpy of larger PAHs is difficult because of their low vapor pressures and in combustion calorimetry, they often result in soot formation. Incomplete combustion can be a significant source of error.

In this regard, estimation methods, *ab initio* quantum mechanical methods, and more recently, density functional theory (DFT) calculations have been used as an independent confirmation of the accuracy of the experimental measurements and often because of lack of available experimental data.

Stein *et al.* [1985STE/FAH, 1977STE/GOL] have proposed an estimation method for the thermochemical properties of PAHs, which extends the additivity procedure of Benson *et al.* [1976BEN, 1969BEN/CRU, 1958BEN/BUS]. Several methods have been reported to solve one specific weakness of the original method proposed by Stein *et al.* [1995POP/HOW, 1993ARM/BIR, 1992HER/NOW, 1990MOI/DOR, 1989MOI/DOR]. Moiseeva *et al.* introduced some changes [1989MOI/DOR] and their group additivity method was later extended for benzenoid PAHs by introducing three new groups for the carbons in five membered rings [1990MOI/DOR]. A new bond-additivity method to estimate the heat of formation of benzenoid PAHs has been proposed by Herndon *et al.* [1992HER/NOW] with additional parameters that take into account the nonplanarity effects that increase with the number of rings in the same bay region, introducing groups for bay regions with five- and six-membered rings. Pope and Howard [1995POP/HOW] and Armitage and Bird [1993ARM/BIR] have introduced a new parameter for a group that belongs to a five-membered ring.

With the advancement of computational capabilities, calculations beyond group additivity methods, such as quantum mechanical calculations on larger molecules, have become increasingly affordable. However, accurate quantum calculations such as the Gn or CBS-n methods are computationally very expensive and PAHs containing more than 15 heavy atoms are still too large for these kinds of calculations. The computational demands of DFT calculations increase in a less drastic way than do *ab initio* methods. In spite of this, it is still not feasible to do DFT calculations on the larger PAHs. Lower level quantum chemical calculations for PAHs have been performed by various groups. Calculated molecular thermochemical properties for PAHs have been determined using semiempirical methods [2004MAR/WOR, 2001POG/AGR, 1998HER/BIE, 1998HAI, 1998NOT/ABB, 1987HIT/SIM]. However, the reliability of the semiempirical results may be questioned; in particular, they do not appear useful in determining the enthalpy of formation of catacondensed benzenoids [2002POG/AGR, 1990HER/CON].

Several self-consistent-field [2002POG/AGR, 1997SCH/DIS, 1992DIS/SCH, 1990PEC/SCH, 1989SCH/PEC] and DFT [2005SIV/TRA, 2005SIV/TRA2, 2002POG/AGR, 1998HER/BIE, 1997SCH/DIS, 1997WIB] calculations, principally at the B3LYP level of theory, have also been used for the calculation of the enthalpies of formation of PAHs. However, analysis of the results obtained from the total energies obtained from computational methods shows that no general method for determination of accurate enthalpies of formation of PAHs has been proposed.

Gn theories at levels G2(MP2) [1999NOT/CAS], G2 [1999NOT/CAS], and G3 [2000NOT/CAS] have been applied by Notario *et al.* to calculate the enthalpies of formation in the gas phase of low molecular weight PAHs. Furthermore, a G3(MP2)//B3LYP study for molecules from benzene to coronene has been carried out by Blanquart and Pitsch [2007BLA/PIT]. In some of these studies [1999NOT/CAS, 2007BLA/PIT], different group corrections are applied to account for systematic errors in the computations.

Sivaramakrishnan *et al.* [2005SIV/TRA] proposes the use of a systematic procedure, namely, the ring conserved isodesmic reaction method. This method is based on the construction of isodesmic reactions preserving aromaticity and minimizing the numbers of molecules involved by decomposing PAHs into an appropriate number of benzene rings. Sun *et al.* [2007SUN/YAO] employed hyperhomodesmotic reactions where strain and resonance energies are balanced in reactants and products in order to achieve more reliable enthalpies of formation.

There also exist many approaches to calculate the enthalpy of formation of PAHs using calculated *ab initio* or semiempirical energies combined with group additivity parameter contributions. Recently, a self-consistent estimation method for the calculation of thermochemical properties of PAHs using DFT calculations [2004YU/SUM] at the B3LYP/6-31G(d) level of theory has been reported that provides values for enthalpies of formation, entropies, and heat capacities of 139 PAHs. This new estimation method is a systematic extension of the atom-centered group method originally proposed by Benson [1976BEN]. It is based on bond-centered groups that define bonds linking two atom-centered groups and specifies the size of the rings to which the atoms belong. It also includes a term to describe the resonance energy.

The main problem associated with these estimations and computational approaches is the insufficient number of experimental benchmark values available for comparison. The quality of any computation can be assessed only by comparison of its results to experimental data. If for a selected compound, different experimental thermochemical values from literature can be located, the quality of the assessment is compromised. In addition, some recent experimental values have gone unnoticed by a number of investigators working in the field.

This publication is the result of the work of the International Confederation for Thermal Analysis and Calorimetry working group on "Thermochemistry" during the period 2000–2007. The purpose of this work is to provide, whenever possible, tables of critically evaluated chemical thermodynamic properties of PAHs. The most recent review of the thermochemistry of PAHs was reported by Slayden and Liebman [2001SLA/LIE]. Additionally, several compendia of vapor pressures [1997DEL] and phase change enthalpies [2000SHI/MA] of PAHs have been also published in the past few decades.

In the current work, the tables contain evaluated values for the enthalpies of combustion and formation, both in the condensed and gas phases, fusion, vaporization, and sublimation of neutral PAHs. The first molecule analyzed is the parent compound benzene, the quintessential and archetypal parent molecule that exhibits the property of aromaticity in all of its many structural and chemical manifestations [2001SLA/LIE]. The target compounds examined are the neutral polycyclic aromatic carbocycles containing σ linked polyphenyls, catacondensed PAHs wherein each fused carbon atom is common to no more than two rings, pericondensed PAHs that have carbon atoms common to three benzenoid rings, and PAHs with fused five-membered rings, from benzene to $C_{42}H_{28}$. A few alkyl substituted or linked aromatic molecules such as toluene, diphenylmethane, triphenylmethane, and tetraphenylmethane are also included. Although this work focused on the original literature, other compilations of thermochemical data have also been consulted [2005AFE/LIE, 2003CHI/ACR, 2002CHI/ACR, 2000SHI/MA, 1999SAB/XU, 1997DEL, 1987STE/MAL, 1986PED/NAY, 1985MAJ/SVO, 1977ZWO, 1971WIL/ZWO, 1970COX/PIL, 1956HAN].

2. Enthalpies of Formation

The enthalpies of formation in the gas phase are generally calculated by combining condensed phase enthalpies of formation with enthalpies associated with phase changes at the temperature of reference, $T=298.15$ K.

High-precision combustion calorimetry is considered to be the best technique to determine the enthalpy of formation of organic compounds. Combustion energies have been measured for many years and different techniques have been developed to do so. These techniques are described by a number of acronyms that are used throughout the tables. A summary of these acronyms and their meanings can be found in Table 305 in the Appendix. From the energy released in the combustion reaction, the standard enthalpy of formation in the condensed state, $\Delta_f H_m^o$(cd) can be calculated.

The heat released in the combustion calorimeter has to be produced for a well defined reaction. This means that calculation of the amount of reaction from the mass of substance put into the calorimeter presupposes that the substance is pure [1970COX/PIL]. The degree of purity of the sample used in a measurement of the heat of combustion can significantly affect the overall accuracy of the measurement as follows: (a) the use of an impure compound implies that the substance is not in its standard state, (b) an erroneous molecular weight may be applied if the impurity is not isomeric, and (c) the heat of combustion will reflect the potential energy change due to the combustion of the impurity as well.

For calculating the number of moles of reaction, it is necessary to verify that complete combustion has been achieved and that only CO_2 and H_2O are produced. The absence of carbon (soot) is verified by visual inspection both of the crucible and on the walls of the combustion bomb. The absence of CO can be determined using Dräger tubes (sensitivity level $\approx 1 \times 10^{-6}$). Some authors have based the results of their experiments on quantitative recovery of the CO_2 formed. The term “amount reactant” in the tables that follow indicates how the extent of combustion was determined. The term “m” is used if the determination of the extent of reaction was determined from the mass of reactant; the term “CO_2” is used if the determination is from the mass of carbon dioxide formed in the combustion of the reactant. When soot is formed, its massic energy of combustion must be taken into account as indicated by Rossini [1956ROS]. Frequently, the most challenging part of a calorimetric experiment is the combustion process since the overall accuracy of the experiment may well be limited by the completeness of the chemical reaction [1970COX/PIL].

Auxiliary materials (oil, vaseline, benzoic acid, etc.) are sometimes used to obtain complete combustion [1979COX]. In these instances, a correction related to the amount of the auxiliary substance used and its heat of combustion must be included in the calculations.

In combustion calorimetry, accuracy and not precision is most important. The reported precision of a set of measurements refers only to random errors and, in accordance with normal thermochemical practice, the uncertainty assigned is twice the overall standard deviation of the mean and includes the uncertainties in calibration and in the values of the auxiliary quantities [1979OLO]. When high precision is achieved, systematic errors may be considerably larger than random errors, leading to an inaccuracy that it is much larger than the uncertainty interval. To check the accuracy of the results obtained, reference materials containing the same elements and in the same physical state as the compounds being investigated must be used [1999SAB/XU].

When a substance is burned, the energy released may differ significantly from that which would occur if the combustion reaction was performed under standard conditions. This problem was studied by Washburn [1933WAS], who analyzed what corrections must be applied to the calorimetric data in order to obtain values of the change in the internal energy under standard conditions. In high-precision combustion calorimetry, it has become standard practice to apply these corrections. All these considerations have been taken into account in the evaluation of the condensed phase enthalpies of combustion data reported in this work. The work that has been reviewed has been reported over the time period from 1878 to the present.

The enthalpies of formation in the condensed state, $\Delta_f H_m^o$(cd), for PAHs have been calculated from the combustion reaction

$$C_aH_b + (a + b/2)O_2 \rightarrow aCO_2 + b/2H_2O \tag{1}$$

using the values reported for CODATA [1989COX/WAG] for the enthalpies of formation of CO_2 and H_2O in their standard states at T=298.15 K,

$$\Delta_f H_m^o(H_2O,\ l) = -(285.830 \pm 0.040)\ \mathrm{kJ\ mol^{-1}},$$

$$\Delta_f H_m^o(CO_2,\ g) = -(393.51 \pm 0.13)\ \mathrm{kJ\ mol^{-1}}.$$

The uncertainties of the enthalpy of formation of PAHs calculated from different values to those reported in CODATA have been recalculated. The new values are given in brackets in the tables.

Most of the early thermochemical measurements reported in the literature have been reported in kcal mol^{-1}. Energy units reported in this review are in kJ mol^{-1}, where 1 cal =4.184 J. All temperatures are reported in K.

3. Phase Change Enthalpies

The phase change enthalpy data evaluated in this section have been reported over the time period from 1917 to the present during which time several temperature scales have been employed. No attempt was made to correct these data to the present temperature scale, ITS-90. Vaporization enthalpies and sublimation enthalpies have been measured for many years and numerous techniques have been developed to do so. Generally, these techniques can be categorized into two groups, calorimetric techniques, in which the phase change enthalpy is measured directly, and techniques in which vapor pressure is measured as a function of temperature. These techniques are described by a number of acronyms that are used throughout the tables. A summary of these acronyms and their meanings can be found in Table 305 of the Appendix.

Phase change enthalpies are temperature dependent. Several methods have been reported to adjust these values with temperature [2003CHI/ACR, 2002CHI/ACR, 1998CHI]. The question arises as to whether to use experimental $C_{p,m}$(s) and $C_{p,m}$(l) data for these adjustments or empirical relationships developed for this purpose. An argument can be made for either case. It is important to note that while experimental $C_{p,m}$(s) and $C_{p,m}$(l) data are available for many of the PAHs, these properties are temperature dependent and correction of sublimation and vaporization and enthalpies to $T=298.15$ K also requires $C_{p,\mathrm{m}}(\mathrm{g})$ of the gas phase, which needs to either be estimated or calculated. Adjusting fusion enthalpies to $T=298.15$ K also requires $C_{p,\mathrm{m}}(\mathrm{l})(298\ \mathrm{K})$ values which are not available for PAHs that are solids at room temperature. As a means of circumventing the lack of sufficient available data, empirical relationships have been developed to adjust solid and liquid phase change enthalpies with temperature. The empirical relationship used to adjust each respective phase change and how it was derived is discussed below.

3.1. Vaporization Enthalpies

Adjustments to $T=298.15$ K from the mean temperature of measurement have been included. In many instances, the temperature adjustments applied by the authors have been used. In other cases as noted in the tables, the temperature adjustments have been applied using Eq. (2) [1993CHI/HOS]. This equation has been derived to model the differences in heat capacity between the liquid and gas phases; it has been derived by correlating vaporization enthalpy differences measured at temperature T and generally at $T=298.15$ K with the estimated heat capacity of each corresponding compound at $T=298.15$ K for which reliable vaporization data are available. The vaporization enthalpy data used were obtained from the critical review and data compilation of Majer and Svoboda [1985MAJ/SVO]. It has been found to provide satisfactory results for adjustments ranging from approximately $T=500$ to 250 K [1998CHI, 1998CHI/ACR]. The adjustments have been generally applied from the mean temperature of measurement, $\bar{T}$, to 298.15 K. Adjustments for temperatures above $T=500$ K should be viewed with some caution:

$$\begin{aligned}\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})/\mathrm{kJ\ mol^{-1}} &= \Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(\bar{T}/\mathrm{K}) + \{10.58 \\ &\quad + 0.26[C_{p,\mathrm{m}}(\mathrm{l})](298.15\ \mathrm{K})_{\mathrm{estd}}/\mathrm{J\ mol^{-1}\ K^{-1}}\} \\ &\quad \times(\bar{T}/\mathrm{K}-298.15)/1000. \qquad (2)\end{aligned}$$

The term $[C_{p,\mathrm{m}}(\mathrm{l})]_{\mathrm{estd}}/\mathrm{J\ mol^{-1}\ K^{-1}}(298.15\ \mathrm{K})$ refers to the molar heat capacity of the liquid phase at $T=298.15$ K; this was estimated by group additivity [1993CHI/HES]. An uncertainty of 16 J mol^{-1} was associated with the bracketed term in Eq. (2) [1993CHI/HOS]. This was combined with the standard deviation ($\pm 2\sigma$) associated with the experimental measurements in assessing the total uncertainty at $T=298.15$ K. The group values used to derive heat capacity estimates are summarized in the Appendix in Table 306.

3.2. Sublimation enthalpies

Sublimation enthalpies adjusted to $T=298.15$ K are also provided. These adjustments are from the mean temperature of measurement to $T=298.15$ K. In some instances, the temperature adjustments applied by the authors reporting the work are included. In other cases as noted in the tables, temperature adjustments have been applied using Eq. (3). This equation has also been derived by correlating sublimation enthalpy differences measured at temperature T and generally at $T=298.15$ K with the estimated heat capacity of each corresponding crystalline compound at $T=298.15$ K [1998CHI, 1993CHI/HOS, 1993CHI/HES]. Unlike vaporization enthalpy data, much less critically evaluated sublimation enthalpy data are available. As a consequence, a larger uncertainty is associated with this adjustment. Some compensation is afforded by the fact that temperature adjustments of sublimation enthalpies are generally smaller than the corresponding adjustments for vaporization enthalpies:

$$\begin{aligned}\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})/\mathrm{kJ\ mol^{-1}} &= \Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(\bar{T}/\mathrm{K}) \\ &\quad + \{0.75 + 0.15[C_{p,\mathrm{m}}(\mathrm{s})(298.15\ \mathrm{K})]_{\mathrm{estd}}/\mathrm{J\ mol^{-1}\ K^{-1}}\} \\ &\quad \times(\bar{T}/\mathrm{K}-298.15)/1000. \qquad (3)\end{aligned}$$

The term $[C_{p,\mathrm{m}}(\mathrm{s})(298.15\ \mathrm{K})]_{\mathrm{estd}}$ refers to the molar heat capacity of the solid phase at $T=298.15$ K and was estimated using a group additivity method [1993CHI/HES]. This equation has been found to give satisfactory results for temperatures up to approximately $T=500$ K [1998CHI, 1998CHI/HES]. Group values used in these estimations are also summarized in the Appendix in Table 306. When using Eq. (3), an uncertainty equal to one-third the magnitude of the total temperature adjustment was arbitrarily assumed and this uncertainty was combined with the uncertainty associated with the experimental measurements to assess the total uncertainty in $\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$. All uncertainties reported in the tables below represent two standard deviations unless noted otherwise. In some cases it was not clear whether the uncertainty reported by the authors represented two standard deviations.

As an internal check on the mutual reliability of all the experimental phase change enthalpies, sublimation enthalpies have also been calculated whenever possible from the sum of the experimental vaporization and fusion enthalpies according to

$$\begin{aligned}\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K}) &= \Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K}) \\ &\quad + \Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K}). \qquad (4)\end{aligned}$$

Equation (4) is a thermodynamic equality if the enthalpies compared are referenced to the same temperature.

3.3. Fusion Enthalpies

Fusion enthalpies were adjusted from T_{fus} to $T=298.15$ K by combining Eqs. (2) and (3). It should be noted that when Eq. (2) is subtracted from Eq. (3), the heat capacity of the gas phase common to both cancels and the remainder results in the difference in molar heat capacity between the solid and liquid phases, $\Delta Cp(\mathrm{cr,l})$, Eq. (5). Equation (5) has been successfully used in combination with Eq. (4) [2004BAS/CHI, 1998CHI/HES]. An uncertainty equal to one-third the magnitude of the total temperature adjustment was arbitrarily assigned to this adjustment and this was combined with the uncertainty associated with the experimental measurements ($\pm 2\sigma$) in assessing the total uncertainty in $\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$. The uncertainties associated with measurements adjusted to $T=298.15$ K were calculated according to Eq. (6) where σ_T represents the uncertainty associated with the experimental measurement made at temperature T and the term $\sigma_{\Delta Cp[T-298.15\ \mathrm{K}]}$ represents the standard deviation associated with the temperature adjustment. The uncertainty is generally not expressed in cases where there is none associated with the experimental measurements:

$$\begin{aligned}\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}&(298.15\ \mathrm{K})/\mathrm{kJ\ mol^{-1}}\\ &= \Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}}) + \Delta_{\mathrm{trans}}H_{\mathrm{m}}(T_{\mathrm{trans}})\\ &\quad \times[0.15C_{p,\mathrm{m}}(\mathrm{cr})_{\mathrm{estd}} - 0.26C_{p,\mathrm{m}}(\mathrm{l})_{\mathrm{estd}} - 9.83]\\ &\quad \times(T_{\mathrm{fus}}/\mathrm{K} - 298.15)/1000, \end{aligned} \tag{5}$$

$$\pm 2\sigma_{298.15\ \mathrm{K}} = [(2\sigma_T)^2 + (2\sigma_{\Delta C_p[T-298.15\ \mathrm{K}]})^2]^{0.5}. \tag{6}$$

Many compounds do not exhibit solid-solid phase transitions. For those compounds that do, the enthalpy of the transition also needs to be included in the total solid-liquid phase change enthalpy, $\Delta_{\mathrm{tpce}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ if this property is being used to estimate $\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ and the sublimation enthalpy was measured at temperatures below T_{trans}. If the sublimation enthalpy was measured above T_{trans}, Eq. (4) can be used directly. For compounds melting below $T=298.15$ K, $\Delta_{\mathrm{trans}}H_{\mathrm{m}}(T_{\mathrm{trans}})$ was not included in the calculation of $\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$.

3.4. Estimated Properties

In many instances, there are not sufficient experimental data to construct a thermochemical cycle as required by equation Eq. (4). Consequently, in addition to experimental data, estimated properties are also included in the tables for comparison. These properties were estimated according to the protocol described in previous work [2003CHI/ACR2]. Vaporization enthalpies were estimated using Eq. (7). The two parameters in Eq. (7), n_c and n_q, refer to the total number of carbons and the total number of quaternary sp^3 hybridized carbon atoms:

$$\begin{aligned}\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})/\mathrm{kJ\ mol^{-1}} &= (4.69 \pm 0.8)(n_c - n_q)\\ &\quad + (1.3 \pm 0.2)n_q + (3.0 \pm 0.2). \end{aligned} \tag{7}$$

Equation (7) has been shown to model vaporization enthalpies of liquid hydrocarbons containing up to 15 carbon atoms easily and accurately. This equation has been found to underestimate the vaporization enthalpies of larger hydrocarbons [1995CHI/HES]. When combined with estimated fusion enthalpies, this equation has been found to provide reasonable estimates of sublimation enthalpies [1998CHI]. It has been found empirically that fusion enthalpies estimated at the melting temperature when combined with vaporization enthalpies at $T=298.15$ K give the best estimates of $\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$. Fusion enthalpies have been estimated using a group additivity approach described previously [2003CHI/ACR2]. The method involves the estimation of the total phase change entropy, $\Delta_{\mathrm{tpce}}S$, in going from a rigid solid at 0 K to an isotropic liquid at the melting point. Multiplication of $\Delta_{\mathrm{tpce}}S$ by the experimental melting point provides $\Delta_{\mathrm{tpce}}H_{\mathrm{m}}^{\mathrm{o}}$, which for most substances is equivalent to the fusion enthalpy. Molecules exhibiting liquid crystalline behavior are overestimated by this method. For most of the PAH examined, the estimation of $\Delta_{\mathrm{tpce}}S$ involves the sum of a few group values. For molecules such as biphenylene, acenaphthene, and related molecules containing four-, five-, or six-membered saturated rings, the estimations require the use of a ring equation. The equations and group values used in estimating total solid-liquid phase change enthalpies for PAHs are included in the Appendix as Tables 307 and 308. The protocol used is described in 2003CHI/ACR2, 1998CHI/ACR.

4. Evaluation of the Data

The data collected in this report summarize thermochemical data found in the literature on PAHs from 1878 to the present. For some compounds, only one experimental measurement is available and this value could not be evaluated because of lack of sufficient data for similar measurements. In cases where there is sufficient data present, a variety of criteria was used in the selection of the recommended value. However it was not possible to apply these criteria uniformly in each evaluation. In some cases, there is very little experimental work reported. In other cases, the precision associated with some of the measurements is not available. Many of the measurements were performed on materials characterized by a physical property such as melting point but lack an independent quantitative assessment of purity. Some literature results fail to report substantial experimental information. In general, depending on the amount of available information, these results were weighed less heavily. Also considered in this assessment is the track record of the laboratory reporting the measurements. Generally, if a physical property was not reported in the reference, this is indicated by the acronym “na.” In a few cases, this term is also used if the property was not available to us in a timely fashion or because the article was in a language with which we lacked familiarity. Compounds previously evaluated as standards for calorimetry were generally not evaluated further [1999SAB/XU]. In these cases, the literature values used in generating the recommended value are summarized and other available data regarding the measurement are tabulated in a supplemental table.

It was also sometimes necessary to evaluate the vapor pressure–temperature data reported by using the Clausius Clapeyron relationship and to assign uncertainties. Probable errors were assigned from the uncertainty associated with the slope calculated from a linear regression analysis. The “Handbook of the Thermodynamics of Organic Compounds,” by Stephenson and Malanowski [1987STE/MAL], was a useful source of vaporization enthalpy information provided in the form of Antoine constants. Unfortunately, references to the original literature data are not provided.

Vaporization enthalpies were calculated from the Antoine equation [Eq. (8)] reported in this compendium using Eq. (9). In these and in a few other instances, the mean temperature chosen, $\bar{T}$, was a temperature at least 15 K within the range of the Antoine constants. In cases where the mean temperature is quite different from $T=298.15$ K, the mean temperature was chosen so as to minimize the temperature adjustment necessary to convert the vaporization enthalpy to $T=298.15$ K. Data evaluated from this source were usually not weighed as heavily as data where the original reference was available:

$$\log p/\text{kPa} = \text{A} - \text{B}/(\text{C} + T), \tag{8}$$

$$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(\bar{T}) = 2.303\text{RB}[\bar{T}/(\bar{T} + \text{C})]^2. \tag{9}$$

Here, A, B, and C are constants, while R is the gas constant. Standard enthalpies are not effected by the selection of standard pressure, although the values had been derived on the basis of the value, $p_o=101.325$ kPa; the IUPAC recommendation in 1981 for standard pressure is $p_o=100$ kPa. The standard deviation of the mean was calculated according to Eq. (10) where N refers to the number of measurements and d_i represents the difference of an individual measurement from the mean:

$$\pm 2SD_M = 2[(\Sigma d_i^2)/N(N-1)]^{1/2}. \tag{10}$$

5. Recommendations

As pointed out above, frequently there are not enough data in literature to allow the comparison of identical measurements from different laboratories or to construct thermochemical cycles and thus recommend enthalpic values for the various phase changes with a high degree of confidence. As a consequence, the thermochemical data included in the tables are either recommended, suggested, or not qualified. Recommended data are ranked the highest followed by suggested data. One criterium used in identifying suggested data for phase change enthalpies was whether it was possible to construct a thermochemical cycle and whether agreement between the direct measurement and the value calculated by the thermochemical cycle was within the expressed uncertainty. Data that are not qualified simply represents data on compounds where any further evaluation was not possible, usually because of lack of supporting or complementary information. In a few cases, particularly with the larger hydrocarbons, the literature value appears to disagree substantially with estimated properties. Agreement (or lack of it) with estimated properties was a factor considered but not weighed very heavily, except in cases where a serious discrepancy was observed. The trends observed between calculated and estimated properties are included in the summary and offer the reader the opportunity to compare the quality of the correlations observed between experiment and estimation.

Thermochemical data, as with spectroscopic information, are characteristic of a compound and essential for future re-evaluation as a consequence of changes in accepted values of reference materials or in standard states. Current journal practices encourage authors to submit thermochemical details as supplementary material. While access to this information is currently available, it is not clear whether this practice will continue indefinitely into the future as journals and the publishing industry evolves through acquisitions and mergers. As an example, the American Chemical Society (ACS), a leader in providing on-line access to all of their journals since their inception, still does not provide on-line access to supplementary material published prior to 1990 as part of the cost of the subscription. While this material is currently available from the ACS, there is no guarantee that it will be available in the future in an appropriate format. Until publishers make such assurances, authors should be reluctant to provide these data as supplementary material.

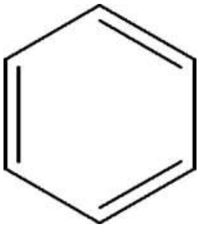
6. Compounds Evaluated

1.	C_6H_6	benzene
2.	C_7H_8	toluene
3.	C_9H_8	indene
4.	C_9H_{10}	indane
5.	$C_{10}H_8$	naphthalene
6.	$C_{12}H_8$	biphenylene
7.	$C_{12}H_8$	acenaphthylene
8.	$C_{12}H_{10}$	acenaphthene
9.	$C_{12}H_{10}$	biphenyl
10.	$C_{13}H_{10}$	fluorene
11.	$C_{13}H_{12}$	diphenylmethane
12.	$C_{14}H_8$	pyracyclene
13.	$C_{14}H_{10}$	anthracene
14.	$C_{14}H_{10}$	phenanthrene
15.	$C_{14}H_{12}$	pyracene
16.	$C_{16}H_{10}$	pyrene
17.	$C_{16}H_{10}$	fluoranthene
18.	$C_{16}H_{14}$	1-phenylnaphthalene
19.	$C_{17}H_{12}$	11*H*-benzo[*a*]fluorene
20.	$C_{17}H_{12}$	11*H*-benzo[*b*]fluorene
21.	$C_{18}H_{12}$	naphthacene
22.	$C_{18}H_{12}$	benz[*a*]anthracene
23.	$C_{18}H_{12}$	triphenylene
24.	$C_{18}H_{12}$	chrysene
25.	$C_{18}H_{12}$	benzo[*c*]phenanthrene
26.	$C_{18}H_{14}$	*p*-terphenyl
27.	$C_{18}H_{14}$	*o*-terphenyl
28.	$C_{18}H_{14}$	*m*-terphenyl
29.	$C_{18}H_{14}$	5,12-dihydrotetracene
30.	$C_{19}H_{16}$	triphenylmethane
31.	$C_{20}H_{10}$	corannulene
32.	$C_{20}H_{12}$	perylene
33.	$C_{20}H_{12}$	benzo[*a*]pyrene
34.	$C_{20}H_{12}$	benzo[*e*]pyrene
35.	$C_{20}H_{12}$	benzo[*k*]fluoranthene
36.	$C_{20}H_{12}$	benz[*e*]acephenanthrylene
37.	$C_{20}H_{14}$	9-phenylanthracene
38.	$C_{22}H_{12}$	benzo[*ghi*]perylene
39.	$C_{22}H_{14}$	benzo[*b*]triphenylene
40.	$C_{22}H_{14}$	dibenz[*a*,*h*]anthracene
41.	$C_{22}H_{14}$	pentacene

42.	$C_{22}H_{14}$	picene
43.	$C_{22}H_{14}$	1,2:6,7-dibenzophenanthrene
44.	$C_{24}H_{12}$	coronene
45.	$C_{24}H_{14}$	naphtho[1,2,3,4-*def*]chrysene
46.	$C_{24}H_{14}$	dibenzo[*b*,*def*]chrysene
47.	$C_{24}H_{14}$	benzo[*r*,*s*,*t*]pentaphene
48.	$C_{24}H_{14}$	dibenzo[*fg*,*op*]naphthacene
49.	$C_{24}H_{18}$	1,3,5-triphenylbenzene
50.	$C_{24}H_{18}$	*p*-quaterphenyl
51.	$C_{25}H_{20}$	tetraphenylmethane
52.	$C_{26}H_{16}$	tetrabenzonaphthalene
53.	$C_{26}H_{18}$	9,10-diphenylanthracene
54.	$C_{26}H_{18}$	9,9′-bifluorenyl
55.	$C_{28}H_{14}$	phenanthro[1,10,9,8-*f*,*g*,*h*,*i*]perylene
56.	$C_{28}H_{18}$	9,9′-bianthracene
57.	$C_{28}H_{18}$	9,9′-biphenanthrene
58.	$C_{30}H_{16}$	pyranthrene
59.	$C_{30}H_{22}$	*p*-quinquephenyl
60.	$C_{32}H_{14}$	ovalene
61.	$C_{34}H_{18}$	violanthrene A
62.	$C_{34}H_{18}$	violanthrene B
63.	$C_{34}H_{18}$	isoviolanthrene A
64.	$C_{34}H_{18}$	isoviolanthrene B
65.	$C_{34}H_{18}$	tetrabenzo[*de*,*hi*,*op*,*st*]pentacene
66.	$C_{42}H_{28}$	5,6,11,12-tetraphenyltetracene

7. Data Sheets and Recommendations

7.1. Benzene



Name	Formula	Registry Number	Molecular Weight
Benzene	C_6H_6	[71-43-2]	78.111 84 g mol^{-1}

7.1.1. Enthalpy of formation (liquid)

TABLE 1. Standard enthalpies of combustion and formation of benzene at $T=298.15$ K

Entry	State	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m(\mathrm{l})$ kJ mol^{-1}	$\Delta_f H^o_m(\mathrm{l})$ kJ mol^{-1}	Reference
1	l	99.98	SMB	na	7	no	m CO_2	-3267.49 ± 0.42 -3267.58 ± 0.50	48.95 ± 0.92	1969GOO/SMI
2	l	99.95	SMB	fpd	11	no	CO_2	-3267.62 ± 0.43^a	49.08 ± 0.90	1970COX/PIL, 1945PRO/GIL, 1947JOH/PRO
3	l	na	SMB	na	6	na	m	-3266.95 ± 0.38	48.41 ± 0.88	1970COX/PIL, 1946COO/MUL
4	g	na	H	na	5	na	P/CO_2	-205.27 ± 0.63^b	48.1 ± 1.0^c	1970COX/PIL, 1936KIS/RUH

[a] Value at $T=301.15$ K.

[b] Enthalpy of hydrogenation in the gas phase.

[c] The enthalpy of formation in the liquid phase has been calculated using the enthalpy of hydrogenation in the gas phase reported in the article in combination with the enthalpy of formation in the gas phase of cyclohexane [1986PED/NAY] and the value for the enthalpy of vaporization of benzene recommended in the present work (*vide infra*).

Recommendation

$\Delta_f H^o_m(\mathrm{l}, 298.15\ \mathrm{K})$	49.0 ± 0.9 kJ mol^{-1}	Recommended value	Entries 1 and 2

Evaluation

The recommended value has been calculated as the mean of the results of Good and Smith [1969GOO/SMI] and Johnson *et al.* [1947JOH/PRO], as revised by Cox and Pilcher [1970COX/PIL].

TABLE 2. Additional enthalpies of combustion of benzene in the condensed phase

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H°(\mathrm{l})$ kJ mol^{-1}	Reference
5	na	SMB	na	na	na	na	−3280	2005AFE/LIE, 1948REP/SCH
6	na	SMB	na	na	na	na	−3265	2005AFE/LIE, 1929LAN/BAY
7	na	SMB	na	na	na	na	−3278	2005AFE/LIE, 1925BAR
8	na	SMB	na	9	sucrose	m	−3275.6	1946PRO/JOH, 1920RIC/DAV
9	na	SMB	na	na	na	na	−3247	2005AFE/LIE, 1918GUI
10	na	na	na	na	na	na	−3276.4	1946PRO/JOH, 1915ROT/VON
11	na	SMB	bp	5	sucrose	m	−3266.8	1946PRO/JOH, 1915RIC/BAR
12	na	na	na	na	na	na	−3273.9	1946PRO/JOH, 1910RIC/JES
13	na	na	na	na	na	na	−3257.2	1946PRO/JOH, 1907RIC/HEN
14	na	na	na	na	na	na	−3265.1	1946PRO/JOH, 1889STO/KLE
15	na	na	na	na	na	na	−3267.6	1946PRO/JOH, 1886STO/ROD
16	na	na	na	na	na	na	−3251.7	1946PRO/JOH, 1878BER

7.1.2. Enthalpy of fusion

TABLE 3. Fusion enthalpy of benzene

Entry	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})^{\mathrm{a}}$ kJ mol^{-1}	Purity %	Reference
1	9.30	279.1	9.84	na	1979SMI
2	8.95	278.8	9.5	na	1967PAC
3	9.94	278.6	10.5	na	1948TSC
4	9.87	278.7	10.4	99.93	1948OLI/EAT
5	9.92	278.7	10.5	99.99	1942ZIE/AND
6	9.83	278.7	10.4	na	1931PAR/HUF
7	9.80	278.6	10.4	na	1930HUF/PAR
8	9.88	278.6	10.4	na	1926AND/LYN
10	10.00	278.6	10.6	na	1925MAA/WAL

[a] Fusion enthalpies adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid benzene of 130.8 and 105 J mol^{-1} K^{-1}, respectively.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$	9.90 ± 0.05 kJ mol^{-1}	Recommended value	Entries 4 and 5
$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	10.5 ± 0.2 kJ mol^{-1}	Recommended value	Entries 4 and 5

Evaluation

The fusion enthalpy of benzene has been measured several times. The recommended value is the mean of the two best measurements (entries 4 and 5) evaluated previously by Domalski and Hearing [1996DOM/HEA]. The uncertainty represents two standard deviations of the mean. The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.1.3. Enthalpy of vaporization

TABLE 4. Vaporization enthalpy of benzene as a function of temperature

$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	Reference	$\Delta_{\mathrm{vap}}H_{m}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	Reference
34.09	293.2	1949YAR/FED	30.83	351.8	1983NAT/VIS
33.92	298.15	1985MAJ/SVO	30.76	353.2	1978MAJ/SVO
33.33	307.2	1978TOD/HOS	30.50	360.5	1983NAT/VIS
32.80	318.2	1978MAJ/SVO	30.21	365.7	1983NAT/VIS

TABLE 4. Vaporization enthalpy of benzene as a function of temperature—Continued

$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	Reference	$\Delta_{\mathrm{vap}}H_{m}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	Reference
31.62	338.2	1978MAJ/SVO	29.26	377.6	1978TOD/HOS

Recommendation

$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	33.92 ± 0.06 kJ mol^{-1}	Recommended value	1985MAJ/SVO

Evaluation

The vaporization enthalpy of benzene has been recommended as a standard for vaporization calorimetry [1968MCC/SCO, 1981AMB, 1999SAB/XU]. Majer and Svoboda have critically reviewed the vaporization enthalpy of benzene [1985MAJ/SVO]. The recommended values were determined from a large database originating from a diverse group of laboratories using a variety of different apparatus. A more recent value of 33.74 ± 0.11 kJ mol^{-1}, obtained calorimetrically, has also been reported [1987SAB/ANT]. Vaporization enthalpies for benzene are available from T=293 K to T=478 K. Errors in the recommended value at T=298.15 K are believed to be less than 0.1%. Table 4 provides a summary of some of the available data at different temperatures. The standard enthalpy of vaporization was obtained by adjusting the recommended enthalpy of vaporization at T=298.15 of 33.83 kJ mol^{-1} for the difference between the enthalpies of ideal gas and saturated vapor. The value of 33.92 ± 0.06 kJ mol^{-1}, recommended by Majer and Svoboda [1985MAJ/SVO], is retained.

7.1.4. Enthalpy of sublimation

TABLE 5. Sublimation enthalpy of benzene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	223–279	45.2	264	44.6[a]	AC	na	1987STE/MAL
2	278	45.1	278	44.8[a]	na	na	1984HES
3	183–197	53.9 ± 1.6	193	52.2 ± 1.7	TE	Uvasol	1977DEK/VAN
4	183–197	49.4 ± 0.8	193	47.7 ± 1.0	ME	Uvasol	1977DEK/VAN
5	229–273	45.2	265	44.7[a]	BG	na	1975HA/MOR
6	262–279	45.2 ± 0.05	269	44.7 ± 0.16[a]	na	na	1971WIL/ZWO
7	195–273	45.6	258	44.9[a]	MM	na	1956MIL
8	236–271	46.0	254	46.0[a]	na	na	1947STU

[a] Sublimation enthalpies adjusted to T=298.15 K using Eq. (5) and an estimated heat capacity for solid benzene of 105 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	44.7 ± 0.2 kJ mol^{-1}	Recommended value	Entries 1, 2, 5–7

Evaluation

The recommended value is the mean of all entries other than 3, 4, and 8. The authors of entries 3 and 4 believe their results to be high in an absolute sense. The uncertainty represents two standard deviations of the mean and the average uncertainty associated with the temperature adjustment according to Eq. (6).

7.1.5. Summary

TABLE 6. A summary of experimental and estimated phase change enthalpies for benzene

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.	9.90 ± 0.05	10.5 ± 0.2	33.92 ± 0.06	44.7 ± 0.2	44.4 ± 0.2[a]
estimated	12		31.1		43.1[b]

[a] Hypothetical property.

[b]Sum of the estimated fusion and vaporization enthalpies: estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=44.4\ \mathrm{J\ mol^{-1}\ K^{-1}}$.

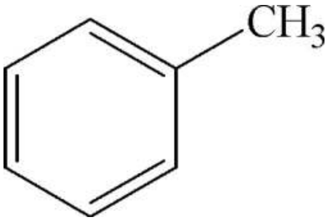
Evaluation

The sublimation enthalpy at $T=298.15$ K calculated according to Eq. (4) is in good agreement with the experimental value.

TABLE 7. A summary of recommended experimental enthalpies of formation of benzene in the condensed and gas phases and for the enthalpy of vaporization

$\Delta_f H^o_m(\mathrm{l}, 298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}} H^o_m(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_f H^o_m(\mathrm{g}, 298.15\ \mathrm{K})$ kJ mol^{-1}
49.0 ± 0.9	33.9 ± 0.1	82.9 ± 0.9

7.2. Toluene



Name	Formula	Registry Number	Molecular Weight
Toluene	C_7H_8	[108-88-3]	92.138 42 g mol^{-1}

7.2.1. Enthalpy of formation (liquid)

TABLE 8. Standard enthalpies of combustion and formation of toluene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m(\mathrm{l})$ kJ mol^{-1}	$\Delta_f H^o_m(\mathrm{l})$ kJ mol^{-1}	Reference
1	99.99 ± 0.01	SMB	mp	11	no	m	-3909.90 ± 0.50	12.01 ± 1.05	1969GOO/SMI
						CO_2	-3910.32 ± 0.50	12.43 ± 1.05	
2	na	SMB	na	7	na	m	-3910.87 ± 0.46	12.98 ± 1.03	1970COX/PIL,1946COO/MUL
3	99.96	SMB	fpd	11	no	CO_2	-3909.95 ± 0.50[a]	12.06 ± 1.05	1945PRO/GIL

[a]Value at $T=301.15$ K.

Recommendation

$\Delta_f H^o_m(\mathrm{l}, 298.15\ \mathrm{K})$	12.04 ± 1.05 kJ mol^{-1}	Recommended value	Entries 1 and 3

Evaluation

The recommended value is the mean of the values obtained from Prosen *et al.* [1945PRO/GIL] and Good and Smith [1969GOO/SMI]. In both cases, the amount of the combustion reaction was calculated from the mass of the toluene burn and analysis of the CO_2 obtained with good agreement.

TABLE 9. Additional enthalpies of combustion of toluene

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m(\mathrm{l})$ kJ mol^{-1}	Reference
4	na	SMB	na	na	na	na	−3938.4	1925BAR
5	na	SMB	bp	6	sucrose	m	−3918.3	1946COO/MUL, 1920RIC/DAV
6	na	SMB	na	na	na	na	−3920.4	1946COO/MUL, 1917RIC/DAV
7	na	na	na	na	na	na	−3916.6	1946COO/MUL, 1915ROT/VON
8	na	SMB	bp	8	sucrose	m	−3921.2	1946COO/MUL, 1915RIC/BAR
9	na	SMB	na	na	na	na	−3933.4	1946COO/MUL, 1906SCH
10	na	SMB	na	na	na	na	−3913.3	1946COO/MUL, 1887STO/ROD

7.2.2. Enthalpy of fusion

TABLE 10. Fusion enthalpy of toluene

Entry	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\ \text{K})^{\text{a}}$ kJ mol^{-1}	Purity %	Reference
1	6.64 ± 0.01	178.2	9.89 ± 1.1	99.999	1962SCO/GUT
2	6.61	178.1	10.38 ± 1.1	na	1931PAR/HUF
3	6.619	178.0	9.88 ± 1.1	na	1929KEL

[a] Fusion enthalpies adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid toluene of 159.2 and 132.6 J mol^{-1} K^{-1}, respectively.

Recommendation

$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$	6.64 ± 0.01 kJ mol^{-1}	Recommended value	Entry 1
$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298.15\ \text{K})$	9.9 ± 1.1 kJ mol^{-1}	Recommended value	Entry 1

Evaluation

The fusion enthalpy of toluene has been reported three times. The recommended value is the value reported by Scott *et al.* [1962SCO/GUT]. The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty at $T=298.15$ K includes an estimate of the uncertainty associated with the temperature adjustment.

7.2.3. Enthalpy of vaporization

TABLE 11. Vaporization enthalpy of toluene as a function of temperature

$\Delta_{\text{vap}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	Reference	$\Delta_{\text{vap}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	Reference
35.5	311	1999EMM/PIC	37.63	298.15	1973SAI/KUS
38.49	296	1998MOK/RAU	33.19	383.8	1962SCO/GUT
33.92	413.0	1993LEE/HOL	31.54	410.1	1962SCO/GUT
38.06	298.15	1985MAJ/SVO	35.65	341.3	1962SCO/GUT
27.07	470.39	1985NAT/VIS	34.53	361.1	1962SCO/GUT
24.02	504.50	1985NAT/VIS	37.99	298.15	1947OSB/GIN
28.4	453.15	1984EUB/CED	38.14	298.15	1943PIT/SCO
35.4	333.15	1984EUB/CED			

Recommendation

$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298.15\ \text{K})$	38.06 ± 0.04 kJ mol^{-1}	Recommended value	1985MAJ/SVO

Evaluation

Majer and Svoboda have critically reviewed the vaporization enthalpy of toluene [1985MAJ/SVO]. Vaporization enthalpies are available from $T=298.15$ K to $T=413.1$ K in their review. Additional data at different temperatures have been reported [1984EUB/CED, 1985MAJ/SVO]. Errors in the values recommended by Majer and Svoboda are believed to be less than 0.25%. Table 11 provides a summary of some of the available data. Vaporization enthalpies at other temperatures can be found in the references. The standard enthalpy of vaporization was obtained by adjusting the recommended enthalpy of vaporization at $T=298.15$ of 38.01 kJ mol^{-1} for the difference between the enthalpies of ideal gas and saturated vapor. The value of 38.06 ± 0.04 kJ mol^{-1}, recommended by Majer and Svoboda, is retained.

7.2.4. Enthalpy of sublimation

Not available.

TABLE 12. A summary of experimental and estimated phase change enthalpies for toluene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)+\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}
expt.	6.64 ± 0.01	9.9 ± 1.1	38.06 ± 0.04	na	48.0 ± 1.1[a]
estimated	8.0		35.8		43.8[b]

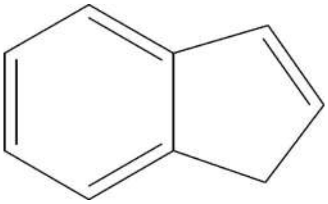
[a] Hypothetical property.
[b] Sum of the estimated fusion and vaporization enthalpies: estimated $\Delta_{tpce}S(T_{fus})=47.1$ J mol^{-1} K^{-1}.

7.2.5. Summary

TABLE 13. A summary of recommended experimental enthalpies of vaporization and formation in the condensed and gas phases for toluene

$\Delta_fH_m^o(1,298.15\ K)$ kJ mol^{-1}	$\Delta_{vap}H_m^o(298.15\ K)$ kJ mol^{-1}	$\Delta_fH_m^o(g,298.15\ K)$ kJ mol^{-1}
12.0 ± 1.1	38.1 ± 0.1	50.1 ± 1.1

7.3. Indene



Name	Formula	Registry Number	Molecular Weight
Indene	C_9H_8	[95-13-6]	116.159 82 g mol^{-1}

7.3.1. Enthalpy of formation (liquid)

TABLE 14. Standard enthalpies of combustion and formation of indene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num of exp.	Aux. Subs.	Amount Reactn.	$\Delta_cH_m^o(1)$ kJ mol^{-1}	$\Delta_fH_m^o(1)$ kJ mol^{-1}	Reference
1	99.7	SMB	fpd	5	mylar	m	-4795.49 ± 1.3	110.58 ± 1.76	1970COX/PIL,1961STU/SIN

Recommendation

$\Delta_fH_m^o(1,298.15\ K)$	110.6 ± 1.8 kJ mol^{-1}	Suggested Value	Entry 1

Evaluation

The equilibrium melting studies made for the authors for the determination of purity indicated purity in the range 99.7–99.9 mole %, although this was not clearly established because of the possibility of solid solution formation with the impurity.

7.3.2. Enthalpy of fusion

TABLE 15. Fusion enthalpy of indene

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H_m^o(298\ K)^a$ kJ mol^{-1}	Method	Purity %	Reference
1	10.20 ± 0.01	271.7	11.18 ± 0.32	AC	99.7+	1961STU/SIN

[a]Fusion enthalpies adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid indene of 187.3 and 143.4 J mol^{-1} K^{-1}, respectively.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$	10.20 ± 0.01 kJ mol^{-1}	Recommended value	Entry 1
$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	11.18 ± 0.32 kJ mol^{-1}	Recommended value	Entry 1

7.3.3. Enthalpy of vaporization

TABLE 16. Vaporization enthalpy of indene

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}\bar{T}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	289–455	44.26[a]	372	48.64[b]	na	na	1987STE/MAL
2	369–457	43.81[a]	413	50.62 ± 1.8	na	na	1987STE/MAL
3	369-406	45.31 ± 0.40[c]	388	50.64 ± 1.5[b]	CE	99.7+	1961STU/SIN
4	290–455	43.91 ± 0.24[c]	372	48.3 ± 1.2[b]	na	na	1947STU
5	329–455	43.86	392	49.4[b]	I	na	1942BUR

[a]Calculated from the Antoine equation.

[b]Vaporization enthalpies adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity for liquid indene of 187.3 J mol^{-1} K^{-1}.

[c]Calculated from the reported vapor pressures over the temperature range indicated.

Recommendation

$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	$50.6\ \pm\ 1.5$ kJ mol^{-1}	Suggested value	Entry 3

Evaluation

Entry 3 is the suggested value. The uncertainty includes the error in the slope as well as the uncertainty ($\pm2\sigma$) associated with the temperature adjustment according to Eq. (6).

7.3.4. Enthalpy of sublimation

Not available

7.3.5. Summary

TABLE 17. A summary of experimental and estimated phase change enthalpies for indene

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.	10.20 ± 0.01	11.18 ± 0.32	50.6 ± 1.5		61.8 ± 1.5[a]
estimated	11.6		45.2		56.8[b]

[a]Hypothetical property.

[b]Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=42.7$ J mol^{-1} K^{-1}.

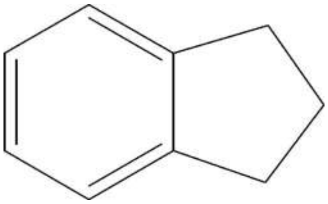
TABLE 18. A summary of experimental enthalpies of vaporization and formation in the condensed and gas phases for indene

$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(1,298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{g},298.15\ \mathrm{K})$ kJ mol^{-1}
110.6 ± 1.8	50.6 ± 1.5	161.2 ± 2.3

Evaluation

Dolliver *et al.* determined the total hydrogenation of indane and indene to form hydrindane in the gas phase at 373 K from which the enthalpy of hydrogenation of indene to indane can be calculated by difference [1937DOL/GRE]. The value was extrapolated to $T=298.15$ K by using Kirchoff's equation [1980HIL/MOR] giving a value of −99.5 kJ mol^{-1}, in good agreement with the value obtained using the values suggested in this work for the enthalpy of formation in the gas phase for both indane and indene $-(100.2\pm 3.1)$ kJ mol^{-1}. The enthalpy of hydrogenation of indane to indane in the gas phase has also been experimentally determined at room temperature by Hill *et al.* [1980HIL/MOR] obtaining a value of $-(98.9\pm 1.4)$ kJ mol^{-1}, again consistent with the value calculated with the data suggested in the present work, confirming the reliability of the enthalpies of formation for both indane and indene. Additionally, several equilibrium studies in the gas phase from 572 to 733 K [1969FRY/WEI] and from 648 to 798 K [1950NAI/MUE] have been reported in the literature. Extrapolation of the data determined in this work leads to the values for the enthalpy of the hydrogenation in the gas phase at $T=298.15$ K of -96.2 kJ mol^{-1} [1969FRY/WEI] and -90.5 kJ mol^{-1} [1950NAI/MUE] lower than the one obtained with the evaluated data. This discrepancy could be due to the large temperature range used in the extrapolation of the data.

7.4. Indane



Name	Formula	Registry Number	Molecular Weight
Indane	C_9H_{10}	[496-11-7]	118.1757 g mol^{-1}

7.4.1. Enthalpy of formation (liquid)

TABLE 19. Standard enthalpies of combustion and formation of indane at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m(\mathrm{l})$ kJ mol^{-1}	$\Delta_f H^o_m(\mathrm{l})$ kJ mol^{-1}	Reference
1	99.98	SMB	na	8	paraffin oil	m CO_2	-4982.47 ± 1.38	11.73 ± 1.82	1971GOO
2	99.89	SMB	fpd	5	mylar	m	-4981.64 ± 1.97	10.90 ± 2.30	1970COX/PIL,1961STU/SIN

Recommendation

$\Delta_f H^o_m(\mathrm{l},298.15\ \mathrm{K})$	11.7 ± 1.8 kJ mol^{-1}	Recommended value	Entry 1

Evaluation

The value selected is the one given by Good [1971GOOD], where the amount of the combustion reaction was calculated from the mass of the indane burned and analysis of the CO_2 obtained with good agreement. This value is also within the respective uncertainty intervals with the value given by Stull *et al.* [1961STU/SIN].

7.4.2. Enthalpy of fusion

TABLE 20. Fusion enthalpy of indane

Entry	$\Delta_{trans}H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H^o_m(298\ \mathrm{K})^a$ kJ mol^{-1}	Method	Purity %	Reference
1	0.78	73.8	8.6 ± 0.1	221.8	11.4 ± 1.0	AC	99.89	1961STU/SIN

[a] Fusion enthalpies adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid indane of 195.5 and 160.8 J mol^{-1} K^{-1}, respectively.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	8.6 ± 0.1 kJ mol^{-1}	Recommended value	Entry 1
$\Delta_{fus}H^o_m(298.15\ K)$	11.4 ± 1.0 kJ mol^{-1}	Recommended value	Entry 1

Evaluation

This value is recommended by Dolmalski and Hearing [1996DOM/HEA]. The uncertainty at $T=298.15$ K includes two standard deviations of the measurement and the uncertainty associated with the temperature adjustment according to Eq. (6)

7.4.3. Enthalpy of vaporization

TABLE 21. Vaporization enthalpy of indane

Entry	T_{Range} K	$\Delta_{vap}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H^o_m(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	382–451	41.94 ± 0.02	415	49.13[c]	VFC	99.94	1981HOS/SCO
2	374–466	42.83 ± 0.18	400	49.0 ± 0.4	CE	99.94	1978OSB/SCO
3	355–393	44.75 ± 0.2[a]	374	49.4 ± 1.2[d]	CE	99.7	1976AMB/SPR
4	364–401	44.16 ± 0.05[b]	383	49.4 ± 1.4[d]	CE	99.89	1961STU/SIN

[a] Calculated from the reported vapor pressures over the temperature range indicated.
[b] Calculated from the Antoine equation.
[c] Vaporization enthalpies adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity for liquid indane of 195.5 J mol^{-1} K^{-1}.
[d] Calculated from the relationship between temperature and vaporization enthalpy provided.

Recommendation

$\Delta_{vap}H^o_m(298.15\ K)$	49.2 ± 1.0 kJ mol^{-1}	Recommended value	Entries 1–4

Evaluation

The recommended value is the mean of entries 1–4. The uncertainty includes two standard deviations of the mean as well as an average uncertainty ($\pm 2\sigma$) associated with the average temperature adjustment.

7.4.4. Enthalpy of sublimation

Not available

7.4.5. Summary

TABLE 22. A summary of experimental and estimated phase change enthalpies for indane

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K)+\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}
expt.	8.6 ± 0.1	11.4 ± 1.0	49.2 ± 1.0		60.6 ± 1.4[a]
estimated	10.2		45.2		55.4[b]

[a] Hypothetical property.
[b] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=45.9$ J mol^{-1} K^{-1}.

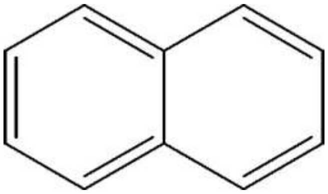
TABLE 23. A summary of recommended experimental enthalpies of vaporization and formation in the condensed and gas phases for indane

$\Delta_fH^o_m(1,298.15\ K)$ kJ mol^{-1}	$\Delta_{vap}H^o_m(298.15\ K)$ kJ mol^{-1}	$\Delta_fH^o_m(g,298.15\ K)$ kJ mol^{-1}
11.7 ± 1.8	49.2 ± 1.0	60.9 ± 2.1

Evaluation

The reliability of the enthalpy of formation in the gas phase is supported by its consistency with the data for the enthalpy of formation of indene and the enthalpy of hydrogenation reported in the literature [1980HIL/MOR, 1937DOL/GRE] (see text above for indene).

7.5. Naphthalene



Name	Formula	Registry Number	Molecular Weight
Naphthalene	$C_{10}H_8$	[91-20-3]	128.17052 g mol^{-1}

7.5.1. Enthalpy of formation (solid)

TABLE 24. Standard enthalpies of combustion and formation of naphthalene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m$(cr) kJ mol^{-1}	$\Delta_f H^o_m$(cr) kJ mol^{-1}	Reference
1	99+	i-SMB	mp,bp	na	no	na	−5160.0 ± 5.2	81.6 ± 5.4	1996BAL/ARZ
2	na	rmb	na	4	no	m	−5165.5 ± 0.8	87.1 ± 1.5	1983MET/KUO
3	na	i-SMB	ea, HPLC	na	na	na	−5153.9 ± 5.2	75.5 ± 5.4	1983HOL2
4	99.98	i-SMB	mp	8	no	m	−5156.4 ± 1.2	79.0 ± 1.8	1977AMM/ELS
5	99.95 ± 0.01	i-SMB	Tfmp	4	no	CO_2	−5156.2 ± 0.3	77.8 ± 1.3	1966COL/PIL
6	na	a-smb	mp,ea	8	no	m	−5147.2 ± 0.5	68.7 ± 1.4	1963MAC/OHA
7	99.97 ± 0.03	i-SMB	fpd	6	no	CO_2	−5157.0 ± 1.6	78.6 ± 2.0	1960SPE/ROS
8	na	i-SMB	na	3	no	m	−5143.4 ± 2.5	64.9 ± 2.8	1952BEN/FAR

Recommendation

$\Delta_f H^o_m$ (cr, 298.15 K)	78.0 ± 1.5 kJ mol^{-1}	Recommended value	Entries 5, 7

Evaluation

Naphthalene is a compound with a high vapor pressure; special care should be taken in the determination of the mass burned. The selected value has been calculated as a weighted average from the results of Speros and Rossini [1960SPE/ROS] and Coleman and Pilcher [1966COL/PIL].

TABLE 25. Ancillary energies of combustion of naphthalene

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r u^o$(cr) J g^{-1}	Reference
9	na	i-SMB	na	na	na	m	−40 224.3 ± 16.4	1970COX/PIL, 1939MAT/ABE
10	na	na	na	na	na	na	−40 258.9	1956HAN, 1939GLI
11	na	i-SMB	na	6	no	m	−40 159.9 ± 11.7	1935HUF/ELL
12	na	SMB	na	5	na	m	−40 162.7 ± 39.0	1970COX/PIL, 1932MIL/ROS
13	na	SMB	na	6	no	m	−40 228.2 ± 11.7	1931KEF
14	na	SMB	na	14	na	m	−40 143.2 ± 39.0	1970COX/PIL, 1931BEC
15	na	na	na	na	na	m	−40 218.5	1931BUR
16	na	SMB	na	6	no	m	−40 225.8 ± 8.4	1927KEF/GUT
17	na	SMB	na	na	na	na	−40 413.4	1925BAR
18	na	na	na	53	na	na	−40 241.5	1931KEF, 1923VER/COO
19	na	na	na	12	na	na	−40 243.6	1931KEF, 1923SCH/FIO
20	na	na	na	13	na	na	−40 148.9	1931KEF, 1922SWI/STA
21	na	na	na	na	na	na	−40 233.9	1931BUR, 1956HAN, 1921HEN
22	na	na	na	8	na	na	−40 171.5	1925BAR, 1920RIC/DAV

TABLE 25. Ancillary energies of combustion of naphthalene—Continued

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r u^{\circ}$(cr) J g^{-1}	Reference
23	na	na	na	na	na	na	−40 211.3	1956HAN, 1917BUR
24	na	na	na	134	na	na	−40 241.1	1931KEF, 1915DIC
25	na	SMB	na	15	no	m	−40 314	1911WRE

7.5.2. Enthalpy of fusion

TABLE 26. Fusion enthalpy of naphthalene

Entry	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	18.99 ± 0.02	353.37	16.8 ± 0.4	AC	99.97	2002CHI/KNI
2	19.02 ± 07	354.1	16.81 ± 0.7	DSC	>98	2001ROJ/ORO
3	18.99	353.4	16.80 ± 0.7	AC	99.97	1993CHI/KNI
4	18.4 ± 0.25	na	na	DSC	na	1983HOL
5	18.91 ± 0.01	353.3	16.73 ± 0.7	AC	99.97	1981DEK/KUI
6	19.4 ± 0.6	353.7	17.2 ± 0.7	DSC		1980MUR/CAV
7	19.06 ± 0.08	353.4	16.9 ± 0.7	AC	99.99	1980AND/CON
8	19.04 ± 0.04	353.4	16.9 ± 0.7	AC	99.99	1979CON
9	18.9 ± 0.4	na	na	DSC	na	1971BEE/LIN
10	18.98 ± 0.01	353.4	16.8 ± 0.7	AC	99.83+	1957MCC/FIN
11	18.81	353.4	16.6 ± 0.7	AC	na	1957MAS
12	20.29	353.5	18.10 ± 0.7[b]	C	na	1933WAR
13	19.20	353.4	17.0 ± 0.7	RC	Mp	1932SPA/THO
14	20.77	353.2	18.59 ± 0.7	C	Mp	1931PAR/HUF

[a] Fusion enthalpies adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid naphthalene of 205 and 157 J mol^{-1} K^{-1}, respectively:

[b] A value of 17.94 kJ mol^{-} is calculated using the temperature dependence of fusion enthalpy reported in this work.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$	19.06 ± 0.08 kJ mol^{-1}	Recommended value	Entry 7
$\Delta_{\mathrm{fus}}\ H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K)	16.9 ± 0.7 kJ mol^{-1}	Recommended value	Entry 7

Evaluation

Naphthalene has been recommended as a standard for fusion enthalpy measurements [1999SAB/XU]. All recent data reported for naphthalene are within the experimental error of the previously recommended value. Lacking new conflicting experimental evidence, the value of Andon and Connett [1980AND/CON], recommended previously, is retained. The fusion enthalpy was adjusted to $T=298.15$ K, as noted above; the uncertainty includes two standard deviations of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.5.3. Enthalpy of vaporization

TABLE 27. Vaporization enthalpy of naphthalene

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(T)$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	60.3 ± 2.1	GC	98+	2006HAF/PAR
2	384–539	48.7 ± 0.3	400	54.8 ± 0.4	E	99.93	1993CHI/KNI
3	353–363	53.2 ± 2.7[a]	358	57.0 ± 3.3[b]	PG	99+	1988SAS/JOS
4	na	54.2 ± 0.8	na	na	DSC	na	1983HOL
5	355–388	50.2 ± 0.15	373	55.0 ± 1.2[b]	DM	99.97	1981DEK/KUI
6	355–490	59 ± 4.0	423	67.0 ± 4.5[b]	DSC	na	1971BEE/LIN
7	353–452	50.6 ± 0.3[a]	369	55.1 ± 1.1[b]	QHG	99.99	1968FOW/TRU

TABLE 27. Vaporization enthalpy of naphthalene—Continued

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(T)$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
8	399–492	48.8 ± 0.6[a]	417	56.4 ± 2.0[b]	P-BP	99.96	1955CAM/ROS
9	360–497	47.2 ± 0.2	429	55.5 ± 1.8	I	na	1923MOR/MUR

[a] Calculated from the Antoine equation.

[b] Vaporization enthalpies adjusted to $T = 298.15$ K using Eq. (2) and an estimated heat capacity for liquid naphthalene of 205 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	55.4 ± 1.4 kJ mol^{-1}	Recommended value	Entries 2, 5, 7-9

Evaluation

The recommended value for the vaporization enthalpy is the mean of all entries other than 1, 3, 4, and 6 in Table 27. The uncertainty represents two standard deviations of the mean and an average uncertainty due to the temperature adjustment calculated according to Eq. (6). Naphthalene has been recommended as a secondary standard for calibrating vaporization calorimeters [1999SAB/XU]. The value recommended presently differs slightly from the previous one in that entry 3 was previously included in the calculation of the mean. Entry 3 has been excluded because the range of temperatures investigated was only 10 K. The recommended value also includes a new entry, entry 9. The recommended value is also consistent with the thermochemical cycle reported in Table 30. Ruzicka *et al.* [2005RUZ/FUL] have carefully examined the phase change properties of napthalene. Their recommendations are discussed below.

7.5.4. Enthalpy of sublimation

TABLE 28. Sublimation enthalpy of naphthalene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	258–313	na		72.44[a]	na	99+	2005RUZ/FUL
2	298	72.7 ± 0.4	298	72.7 ± 0.4	E	99.93	1993CHI/KNI
3	298	70.73 ± 2.1	298	70.73 ± 2.1	C	cg	1987SAB/ANT
4	244–256	72.92 ± 0.74	250	72.9 ± 0.74[b]	SRFG	99.97	1983VAN/JAC
5	271–285	73.9 ± 0.6	278	72.8 ± 0.6[b]	ME	99.95+	1982COL/JIM
6	274–353	na	314	72.51 ± 0.28[b]	DM	99.97	1981DEK/KUI
7	253–273	74.4 ± 1.0	263	72.6 ± 1.2[b]	TE, ME	zrm	1980DEK
8	298	72.5 ± 0.25	298.15	72.5 ± 0.25	na	na	1993LEE/HOL, 1977AMB
9	220–353	73.65 ± 0.3	260	72.5[b]	GS	99.99	1974SIN
10	298	72.05 ± 0.5	298.15	72.05 ± 0.5	C	OAS	1972MOR
11	298	73.0 ± 0.5	298.15	73.0 ± 0.5	C	zrm	1972IRV
12	230–260	74.38	245	72.68 ± 0.66[b]	KG	99.7	1963MIL

[a] See discussion below

[b] Sublimation enthalpies reported at or adjusted to $T = 298.15$ K by Chirico *et al.* [1993CHI/KNI].

Recommendation

$\Delta_{\mathrm{sub}}\ H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	72.6 ± 0.3 kJ mol^{-1}	Recommended value	[1999SAB/XU]

Evaluation

Naphthalene has been repeatedly recommended as a standard for sublimation enthalpy measurements, 72.5 ± 0.25 [1974COX], 72.6 ± 0.3 [1987HEA/SAB], and 72.6 ± 0.6 kJ mol^{-1} [1999SAB/XU]. A summary of sublimation enthalpies of naphthalene measured over the temperature range $T = 280$ K to $T = 340$ K has been reported by Chirico *et al.* [1993CHI/KNI]. A partial listing of values reported at $T = 298.15$ K by these authors is summarized in Table 28 as well as a more recent critical evaluation [2005RUZ/FUL]. A mean value of 72.45 ± 0.4 kJ mol^{-1} is calculated using entries 2–12. The uncertainty represents two standard deviations of the mean. A similar value is recommended by Ruzicka *et al.* (72.44 kJ mol^{-1}, $T = 298.15$ K) in a more recent critical evaluation of a more limited data set. The Recommendation of Ruzicka *et al.* is based on the consistency of vapor pressure and several calorimetric properties measured at the triple point and included results of their own vapor pressure measurements. No uncertainty is provided. If entry 3, which is more than three standard deviations from the mean is omitted, this results in a mean value of 72.6 ± 0.18 kJ mol^{-1} for ten entries. This value is within experimental error to the value recommended previously, 72.6 ± 0.3 kJ mol^{-1} [1999SAB/XU]. In view of the agreement with experimental error of the most recent recommendation with the previous value, there appears to be no compelling experimental evidence to modify the value presently accepted, particularly in view of the absence of any uncertainty associated with the new recommendation. The value recommended in 1987 is retained [1987HEA/SAB]. Recommended vapor pressures and sublimation enthalpies are also provided from $T=150$ to the triple point by Ruzicka *et al.* and should be consulted. Additional experimental sublimation enthalpies can be found in Table 29.

TABLE 29. Ancillary sublimation enthalpy values reported for naphthalene

Entry	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\text{ K})^{\text{a}}$ kJ mol^{-1}	Method	Reference
13	72.70 ± 0.04	298	72.70 ± 0.04	BAG	2006MON/SAN
14	71.70 ± 1.27	298	71.70 ± 1.27	DSC	2001ROJ/ORO
15	88.02 ± 5.0	285	87.7 ± 5.0	DSC	1998BOL/WIE
16	73.7 ± 1.0	298	73.7 ± 1.0	CGC-DSC	1998CHI/HES, 1995HOS
17	71.7	na	na	GS	1995NAS/LEN
18	73.7 ± 2.0	258	72.7 ± 2.0	GS	1994WAN/SHU
19	78.2 ± 2	na	na	GS	1988KHU
20	70.9 ± 0.8	323	71.4 ± 0.9	DSC	1988TOR/BAR
21	72.3 ± 0.8	298	72.3 ± 0.8	DSC	1988TOR/BAR
22	73.4	315	74.1	GS	1986SAT/INO
23	69.9	363	71.5	T	1985MAT/KUW
24	72.3 ± 1.6	312	72.6 ± 1.7	QC	1985GLU/ARK
25	75.8 ± 2.2	303	75.8 ± 2.2	GS	1983SON/ZOL
26	72.6 ± 0.8	na	na	DSC	1983HOL
27	72.4 ± 1.4	298	72.4 ± 1.4	C	1982MUR/SAK
28	76.0 ± 4.0	na	na	DSC	1980MUR/CAV
29	66.3 ± 8.8	280	65.5 ± 8.8	VG	1979CON
30	71.3	293	71.2	GS	1979GOO
31	74.77 ± 1.6	273	74.2 ± 1.7	TE	1977DEK/VAN
32	73.9 ± 0.8	273	73.3 ± 1.0	ME	1977DEK/VAN
33	74.35 ± 3.4	316	74.8 ± 3.5	TSGC	1975CLA/KNO
34	72.5 ± 0.6	298	72.5 ± 0.6	DM	1975AMB/LAW
35	67.8 ± 7.0	280	67.4 ± 7.0	HAS	1975CHI
36	72.7 ± 3.4	289	72.5 ± 3.4	ME	1974RAD/KAT
37	64 ± 1.0	285	63.5 ± 1.1	LE	1973MCE/SAN
38	66.5	na	na	na	1968KAR/RAB
39	73.4	315	74.1	GS	1968SAT/INO
40	72.6 ± 0.2	298	72.6 ± 0.2	TE,ME,DM	1987SAB/ANT, 1963MIL
41	66.8 ± 0.6	280	66.4 ± 0.6	QF	1959AIH
42	69.2	268	68.5	na	1958HOY/PEP
43	72.4	287	71.9	ME	1953BRA/CLE
44	66.5 ± 3.4	298	66.5 ± 3.4	QF	1938WOL/WEG

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid naphthalene of 157 J mol^{-1} K^{-1} in cases where the authors report enthalpies at the mean temperature of measurement.

7.5.5. Summary

TABLE 30. A summary of experimental and estimated phase change enthalpies for naphthalene

	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298\text{ K})^{1}$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\text{ K})+\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}
expt.	19.06 ± 0.08	16.9 ± 0.7	55.4 ± 1.4	72.6 ± 0.3	72.3 ± 1.6
estimated	15.6		49.9		65.5$^{\text{a}}$

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\text{tpce}}S(T_{\text{fus}})=44.2$ J mol^{-1} K^{-1}.

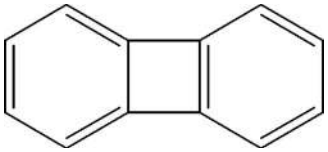
Evaluation

Recommended phase change enthalpies for naphthalene are summarized in Table 30. The sublimation enthalpy calculated according to Eq. (4) is in excellent agreement with the experimental value.

TABLE 31. A summary of recommended experimental enthalpies of sublimation and formation in the condensed and gas phases for naphthalene

$\Delta_f H_m^o(\mathrm{cr}, 298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{sub} H_m^o$ (298.15 K) kJ mol^{-1}	$\Delta_f H_m^o(\mathrm{g}, 298.15\ \mathrm{K})$ kJ mol^{-1}
78.0 ± 1.5	72.6 ± 0.3	150.6 ± 1.5

7.6. Biphenylene



Name	Formula	Registry Number	Molecular Weight
Biphenylene	$C_{12}H_8$	[259-79-0]	152.191 92 g mol^{-1}

7.6.1. Enthalpy of formation (solid)

TABLE 32. Standard enthalpies of combustion and formation of biphenylene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H_m^o$(cr) kJ mol^{-1}	$\Delta_f H_m^o$(cr) kJ mol^{-1}	Reference
1	na	RMB	CO_2 recovery 99.999%	7	no	m, CO_2	−6198.8 ± 0.9	333.4 ± 1.8	1978GOO
2	na	SMB	mp: 383–384 K, ea, IR, UV, CO_2 recovery:99.5/99.7%	5	melinex	CO_2	−6218.7 ± 2.9	353.3 ± 5.9	1962BED/CAR
3	na	SMB	mp:383–384 K	2	filter paper	m	−6198 ± 10	333 ± 10	1955CAS/SPR

Recommendation

$\Delta_f H_m^o$ (cr, 298.15 K)	333.4 ± 1.8 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

There are three available values for the enthalpy of combustion of biphenylene that are spread over 20 kJ mol^{-1}. From the evaluation of the CO_2 produced in the reaction, the suggested value is that given by Good [1978GOO].

7.6.2. Enthalpy of fusion

TABLE 33. Fusion enthalpy of biphenylene

Entry	$\Delta_{fus} H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus} H_m^o(298\ \mathrm{K})^a$ kJ mol^{-1}	Method	Purity mol %	Reference
1	22.6 ± 0.7	385.4	18.7 ± 1.4	DSC	99	2008HAN/NUT

[a] Fusion enthalpies adjusted to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid biphenylene of 235.6 and 174 J mol^{-1} K^{-1}, respectively.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	22.6 ± 0.7 kJ mol^{-1}	Suggested value	Entry 1
$\Delta_{fus}H_m^o(298\text{ K})$	18.7 ± 1.4 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The uncertainty at T=298.15 K includes both the uncertainty associated with the measurement and the temperature adjustment.

7.6.3. Enthalpy of vaporization

TABLE 34. Vaporization enthalpy of biphenylene

Entry	$\Delta_{vap}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H_m^o(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	66.4 ± 1.7	298	66.4 ± 1.7	CGC	99[a]	2008HAN/NUT

[a] The chromatography generally separates any impurities.

Recommendation

$\Delta_{vap}H_m^o$ (298.15 K)	66.4 ± 1.7 kJ mol^{-1}	Suggested value	Entry 1

7.6.4. Enthalpy of sublimation

TABLE 35. Sublimation enthalpy of biphenylene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H_m^o(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	313–453	82.7	na	na	GS	99.9	1995NAS/LEN
2	312–333	104.5	322	105.1[a]	na	na	1989ROR/RUT
3	298	83.8 ± 0.6	298	83.8 ± 0.6	C	99.5+	1972MOR
4	371–381	129.3	376	131.4[a]	na	na	1955CAS/SPR

[a] Sublimation enthalpies adjusted to T=298.15 K using Eq. (3) and an estimated heat capacity for solid biphenylene of 174 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H_m^o(298.15\text{ K})$	83.8 ± 0.6 kJ mol^{-1}	Suggested value	Entry 3

Evaluation

The suggested value is that reported by Morawetz [1972MOR]. No experimental details are provided in 1995NAS/LEN.

7.6.5. Summary

TABLE 36. A summary of experimental and estimated phase change enthalpies for biphenylene

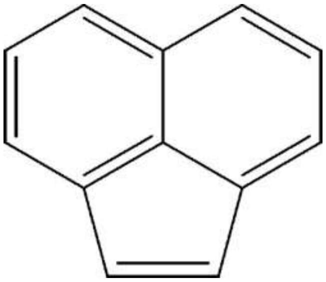
	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\text{ K})$ kJ mol^{-1}	$\Delta_{vap}H_m^o(298\text{ K})$ kJ mol^{-1}	$\Delta_{sub}H_m^o(298\text{ K})$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\text{ K})+\Delta_{vap}H_m^o(298\text{ K})$ kJ mol^{-1}
expt.	22.6 ± 0.7	18.7 ± 1.4	66.4 ± 1.7	83.8 ± 0.6	85.1 ± 2.2
estimated	18.2		59.3		77.5[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})$=47.1 J mol^{-1} K^{-1}.

TABLE 37. A summary of suggested experimental enthalpies of sublimation and formation in the condensed and gas phases for biphenylene

$\Delta_f H_m^o$(cr, 298.15 K)	$\Delta_{sub} H_m^o$(298.15 K)	$\Delta_f H_m^o$(g, 298.15 K)
kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
333.4 ± 1.8	83.8 ± 0.6	417.2 ± 1.9

7.7. Acenaphthylene



Name	Formula	Registry Number	Molecular Weight
Acenaphthylene	$C_{12}H_8$	[208-96-8]	152.191 92 g mol^{-1}

7.7.1. Enthalpy of formation (solid)

TABLE 38. Standard enthalpies of combustion and formation of acenaphthylene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H_m^o$(cr) kJ mol^{-1}	$\Delta_f H_m^o$(cr) kJ mol^{-1}	Reference
1	99.95+	i-smb	GC	7	n-hexadecane (B.D.H.)	m	−6056.2 ± 3.1	190.8 ± 3.5	2002DIO/KIY
2	na	SMB	na	3	no	m	−6059 ± 8	193.6 ± 8.2	1966SAD
3	na	a-RMB	mp 93.0–93.5	6	no	m	−6052.8 ± 4.9	187.4 ± 4.9	1965BOY/CHR

Recommendation

$\Delta_f H_m^o$ (cr, 298.15 K)	190.8 ± 3.5 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The suggested value is the value reported by Diogo *et al.* [2002DIO/KIY]. This value was obtained with a sample of high purity and falls within the mean of the rest of the data.

7.7.2. Enthalpy of fusion

TABLE 39. Fusion enthalpy of acenaphthylene

Entry	$\Delta_{trans} H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus} H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus} H_m^o$(298 K)^a kJ mol^{-1}	Method	Purity %	Reference
1	3.79	116.6				AC	99.99	1994CHE/WES
2			6.94	362.6	3.91	C	na	1996DOM/HEA, 1969SAD/STE

[a] Fusion enthalpies adjusted to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid acenaphthylene of 235.6 and 170.8 J mol^{-1} K^{-1}, respectively.

Recommendation

$\Delta_{\text{fus}} H_m(T_{\text{fus}})$	6.94 kJ mol^{-1}	Suggested value	Entry 1
$\Delta_{\text{fus}} H^{\text{o}}_m$(298.15 K)	4.01 kJ mol^{-1}	Suggested value	Entry 1
$\Delta_{\text{tcpe}} H^{\text{o}}_m$(298.15 K)	7.80 kJ mol^{-1}	Suggested value	Entries 1 and 2

Evaluation

The fusion enthalpy is 6.94 kJ mol^{-1}. The fusion enthalpy was adjusted to T=298.15 K as noted above; the uncertainty associated with the temperature adjustment is ±1.0 kJ mol^{-1}. This value was considered as average quality by Domalski and Hearing [1996DOM/HEA].

7.7.3. Enthalpy of vaporization

TABLE 40. Vaporization enthalpy of acenaphthylene

Entry	$\Delta_{\text{vap}}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{vap}}H^{\text{o}}_m$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	69.1 ± 2.2	298	69.1 ± 2.2	GC	98+	2006HAF/PAR
2	64.6 ± 5.8	298	64.6 ± 5.8	CGC	99[a]	1995HOS

[a] Not relevant to the measurement: the chromatography generally separates any impurities.

Recommendation

$\Delta_{\text{vap}} H^{\text{o}}_m$ (298.15 K)	66.9 ± 4.5 kJ mol^{-1}	Suggested value	Entries 1 and 2

Evaluation

The suggested value is an average of both entries.

7.7.4. Enthalpy of sublimation

TABLE 41. Sublimation enthalpy of acenaphthylene

Entry	T_{Range} K	$\Delta_{\text{sub}}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_m$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	283–323	74.2 ± 8.2	303	74.3 ± 8.2	ME	95+	2008GOL/SUU
2	313–453	77.2	na	na	GS	99.9	1995NAS/LEN
3	283–323	73.2 ± 1.0	303	73.3 ± 1.0[a]	GS	cs[b]	1983SON/ZOL
4	298	73.0 ± 0.7	298	73.0 ± 0.7	C	99.5+	1972MOR
5	286–318	71.1 ± 2.5	306	71.3 ± 2.5[a]	ME	99.0+	1965BOY/CHR

[a] Sublimation enthalpies adjusted to T=298.15 K using Eq. (3) and an estimated heat capacity for solid acenaphthylene of 170.8 J mol^{-1} K^{-1}.
[b] Commercial samples.

Recommendation

$\Delta_{\text{sub}} H^{\text{o}}_m$(298.15 K)	72.5 ± 1.2 kJ mol^{-1}	Recommended value	Entries 3–5

Evaluation

The recommended value is the average of entries 3–5; the uncertainty represents two standard deviations of the mean. No experimental details are provided in 1995NAS/LEN. Entry 1 was not included in the mean because of the large uncertainty.

7.7.5. Summary

TABLE 42. A summary of experimental and estimated phase change enthalpies for acenaphthylene

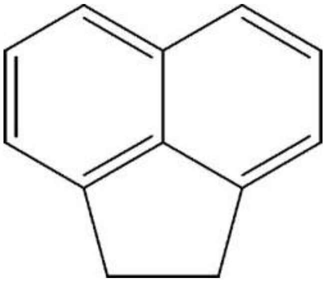
	$\Delta_{fus}H_m(T_{fus})$	$\Delta_{fus}H_m^o(298\ K)$	$\Delta_{vap}H_m^o(298\ K)$	$\Delta_{sub}H_m^o(298\ K)$	$\Delta_{fus}H_m^o(298\ K)+$ $\Delta_{vap}H_m^o(298\ K)$
	kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
expt.	6.94	4.01 ± 1.0	66.9 ± 4.5	72.5 ± 1.2	70.9 ± 4.6
estimated	13.6		59.3		72.9[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=37.6$ J mol^{-1} K^{-1}.

TABLE 43. A summary of suggested enthalpies of sublimation and formation in the condensed and gas phases for acenaphthylene

$\Delta_fH_m^o(cr, 298.15\ K)$	$\Delta_{sub}H_m^o(298.15\ K)$	$\Delta_fH_m^o(g, 298.15\ K)$
kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
190.8 ± 3.5	72.5 ± 1.2	263.2 ± 3.7

7.8. Acenaphthene



Name	Formula	Registry Number	Molecular Weight
Acenaphthene	$C_{12}H_{10}$	[83-32-9]	154.2078 g mol^{-1}

7.8.1. Enthalpy of formation (solid)

TABLE 44. Standard enthalpies of combustion and formation of acenaphthene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_rH_m^o(cr)$ kJ mol^{-1}	$\Delta_fH_m^o(cr)$ kJ mol^{-1}	Reference
1	99	i-smb	GC	6	n-hexadecane (B.D.H.)	m	-6223.3 ± 2.7	72.0 ± 3.1	2002DIO/KIY
2	na	a-RMB	GC	5	no	m	-6221.8 ± 5.0	70.5 ± 5.1	1965BOY/CHR

Recommendation

$\Delta_f H_m^o$ (cr, 298.15 K)	72.0 ± 3.1 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The enthalpy of formation in the condensed phase of entry 1 was calculated on the basis of the massic energy of combustion reported in the supporting information of 2002DIO/KIY.

7.8.2. Enthalpy of fusion

TABLE 45. Fusion enthalpy of acenaphthene

Entry	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	21.5	na	na	DTA	na	1991RAI/SHE
2	21.46 ± 0.02	366.6[b]	18.4 ± 1.1	AC	99.98	1977FIN/MES
3	21.8 ± 0.8	363.1	18.9 ± 1.3	DSC	purum[c]	1973CAS/VEC
4	21.9 ± 0.4	363.2	19.0 ± 1.0	DSC	na	1972WAU/GET
5	20.2	366.4	17.1	C	na	1969SAD/STE

[a] Total phase change enthalpy adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid acenaphthene of 243.8 and 188.2 J mol^{-1} K^{-1}, respectively.

[b] Triple point.

[c] Fluka AG, Buchs, Switzerland.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}$ (T_{fus})	21.46 ± 0.02 kJ mol^{-1}	Recommended value	Entry 2
$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K)	18.4 ± 1.1 kJ mol^{-1}	Recommended value	Entry 2

Evaluation

The fusion enthalpy measured by adiabatic calorimetry as reported by Finke *et al.* [1977FIN/MES] is recommended. The fusion enthalpy at $T=298.15$ K includes an estimate of the uncertainty associated with the temperature adjustment.

7.8.3. Enthalpy of vaporization

TABLE 46. Vaporization enthalpy of acenaphthene

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	70.54	GC	98+	2006HAF/PAR
2	na	na	na	63.9	GC	99	2002LEI/CHA
3	372–512	61.09	366.54	66.18	PG	99.9	1998RUZ/MOK
4	298	66.5 ± 6.0	298	66.5 ± 6.0	CGC	99[a]	1995HOS
5	363–393	60.63 ± 0.4	378	66.5 ± 1.3[b]	PG	99	1995MOK/GUE
6	442–467	55.89[c]	455	67.94[b]	VLRS	99	1991GUP/GUP
7	368–413	54.0[d]	403	64.0[b]	na	na	1987STE/MAL
8	388–552	54.5	470	67.2[b]	na	na	1987STE/MAL
9	368–413	59.8 ± 0.2	391	66.7 ± 1.7[b]	IP	99.98	1975OSB/DOU
10	413–453	54.4 ± 0.2[d]	428	64.0 ± 2.1[b]	I	na	1923MOR/MUR

[a] Not relevant to the method, the chromatography generally separates any impurities.

[b] Vaporization enthalpy adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity of 243.8 J mol^{-1} K^{-1} for liquid acenaphthene.

[c] Calculated from the Antoine constants.

[d] Calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided in the reference over a 30 K range.

Recommendation

$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$ (366.5 K)	61.09 kJ mol^{-1}	Recommended value	Entry 3
$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$ (298.15 K)	66.5 ± 0.2 kJ mol^{-1}	Recommended value	Entries 3–5, 9

Evaluation

Entry 3 is the recommended value at $T=366.5$ K. The value was derived from a critical evaluation of the literature as well as new measurements. The recommended value at $T=298.15$ K is the average of entries 3–5 and 9. The uncertainty represents two standard deviations of the mean as well as the uncertainty associated with the temperature adjustment according to Eq. (6).

7.8.4. Enthalpy of sublimation

TABLE 47. Sublimation enthalpy of acenaphthene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	299–320	78.4 ± 4.4	310	78.7 ± 4.4[a]	ME	99	2008GOL/SUU
2	303–353	82.72	366.5	84.76	PG	99.9	1998RUZ/MOK
3	313–453	83.2	na	na	GS	99.9	1995NAS/LEN
4	293–342	77.1[b]	318	77.7[a]	GS	98	1986SAT/INO
5	303	86.8 ± 1.8	303	86.9 ± 1.8[a]	GS	na	1983SON/ZOL
6	338–366	83.3 ± 0.24	352	84.9 ± 1.7[a]	IP	99.98	1975OSB/DOU
7	342	84.7	342	86.0[a]	ME	na	1974RAD/KAT
8	291–323	86.1	307	86.4[a]	ME	99.9	1965BOY/CHR
9	301	82.1	301	82.2[a]	VG	na	1959AIH
10	283	81.6	283	81.2[a]	na	na	1958HOY/PEP

[a] Sublimation enthalpies adjusted to $T = 298.15$ K using Eq. (3) and an estimated heat for solid acenaphthene of 188.2 J mol^{-1} K^{-1}.

[b] Calculated from the Antoine constants.

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}$ (298.15 K)	84.8 ± 0.4 kJ mol^{-1}	Recommended value	Entry 2

Evaluation

Entry 2 is the recommended value. The value was derived from a critical evaluation of the literature as well as new measurements. The uncertainty represents 0.5% of the value as reported [1998RUZ/MOK]. No experimental details are provided in 1995NAS/LEN.

7.8.5. Summary

TABLE 48. A summary of experimental and estimated phase change enthalpies for acenaphthene

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K}) + \Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.	21.46 ± 0.02	18.4 ± 1.1	66.5 ± 0.2	84.8 ± 0.4	84.9 ± 1.1
estimated	15.0		59.3		74.3[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}}) = 40.8$ J mol^{-1} K^{-1}.

Evaluation

The sublimation enthalpy calculated according to Eq. (4) is in agreement with the experimental value.

TABLE 49. A summary of suggested enthalpies of sublimation and formation in the condensed and gas phases for acenaphthene

$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{cr}, 298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{g}, 298.15\ \mathrm{K})$ kJ mol^{-1}
72.0 ± 3.1	84.8 ± 0.4	156.8 ± 3.1

7.9. Biphenyl

Name	Formula	Registry Number	Molecular Weight
Biphenyl	$C_{12}H_{10}$	[92-52-4]	154.2078 g mol $^{-1}$

7.9.1. Enthalpy of formation (solid)

TABLE 50. Standard enthalpies of combustion and formation of biphenyl at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_c H^o_m$(cd) kJ mol^{-1}	$\Delta_f H^o_m$(cd) kJ mol^{-1}	Reference
1	99.98 ± 0.02	SMB	na	7	polyester	m	−6248.0 ± 2.1	96.8 ± 2.6	1978MON/ROS
2	99.99 ± 0.01	SMB	Tfmp	5	no	CO_2	−6251.8 ± 1.4	100.5 ± 2.1	1966COL/PIL
3	na	smb	mp, ea	5	filter paper	m	−6248.2 ± 4.0	96.8 ± 4.1	1963MAC/OHA
4	na	SMB	mp	10	na	m	−6248.5 ± 1.6	97.2 ± 2.2	1970COX/PIL, 1951PAR/VAU
5	na	SMB	na	3	na	m	−6250.1 ± 8.4	98.8 ± 8.6	1978MON/ROS, 1935BRU
6	na	SMB	na	na	na	na	−6243	92	2005AFE/LIE, 1934WIE/HEY
7	na	SMB	na	na	na	na	−6276 ± 13	125 ± 13	1978MON/ROS, 1925BAR

Recommendation

$\Delta_f H^o_m$(cd, 298.15 K)	98.2 ± 2.5 kJ mol^{-1}	Recommended value	Entries 1–4

Evaluation

The enthalpies of combustion and formation of biphenyl have been reported many times since 1925. From an analysis of the available data, the recommended value has been calculated as the weighted average from the results of entries 1-4.

7.9.2. Enthalpy of fusion

TABLE 51. Fusion enthalpy of biphenyl

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H^o_m$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	18.57 ± 0.06	342.4	16.5 ± 0.7	DSC	99.98	2008SRM
2	18.57 ± 0.01	342.1[b]	16.6 ± 0.7	AC	99.98	1989CHI/KNI
3	18.58 ± 0.3	342.2	16.6 ± 0.7	DSC	99.9+	1983ORO/MRA
4	19.9 ± 0.6	343.3	17.8 ± 1.3	DSC	zr[c]	1982WAS/RAD
5	18.8 ± 0.5	344.1	16.7 ± 0.7	DSC	na	1979SMI
6	18.91 ± 1.0	na	na	DSC	na	1972WAU/GET
7	18.58	343	16.5 ± 0.7	na	na	1950UEB/ORT
8	18.65	341.5	16.7 ± 0.7	RC	na	1932SPA/THO
9	18.6	341.8	16.6 ± 0.7	C	na	1931PAR/HUF

[a] Fusion enthalpy adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid biphenyl of 248.6 and 192 J mol^{-1} K^{-1}, respectively.
[b] Triple point.
[c] Zone refined.

Recommendation

$\Delta_{fus} H_m$ (T_{fus})	18.57 ± 0.004 kJ mol^{-1}	Recommended value	[1999SAB/XU]
$\Delta_{fus} H^o_m$ (298.15 K)	16.6 ± 0.7 kJ mol^{-1}	Recommended value	[1999SAB/XU]

Evaluation

The fusion enthalpy of biphenyl has been recommended as a primary reference material for the calibration of differential scanning calorimeters [1999SAB/XU]. The fusion enthalpy was adjusted to 298.15 K as noted above; the uncertainty includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment. The second entry is the recommended value.

7.9.3. Enthalpy of vaporization

TABLE 52. Vaporization enthalpy of biphenyl

Entry	T_{Range} K	$\Delta_{\text{vap}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	62.5	GC	99+	2002LEI/CHA
2	298	64.3 ± 2.9	298	64.3 ± 2.9	CGC	99[a]	2004CHI/HAN, 1995HOS
3	438–459	54.33[b]	449	65.65[c]	VLRS	99	1991GUP/GUP
4	350–578	53.2 ± 0.1	464	64.9 ± 1.3	IP	99.98	1989CHI/KNI
5	333–393	60.3 ± 0.5[d]	363	65.2 ± 1.5[c]	PG	99	1989SAS/NGU
6	390–563	57.2[b]	405	65.2[c]	na	na	1987STE/MAL
7	396–601	54.9 ± 1.5[d]	417	63.8 ± 3.1[c]	S	99.99	1980NAS/HWA
8	436–595	53.8 ± 0.28[d]	454	65.5 ± 2.5[c]	I	na	1929CHI/PEL

[a] Not relevant to the measurement; the chromatography generally separates any impurities.

[b] Calculated from the Antoine constants.

[c] Vaporization enthalpy adjusted to $T = 298.15$ K using Eq. (2) and an estimated heat capacity of 248.6 J mol^{-1} K^{-1} for liquid biphenyl.

[d] Calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided in the reference.

Recommendation

$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$	64.9 ± 1.3 kJ mol^{-1}	Recommended value	Entry 4

Evaluation

The value reported by Chirico *et al.* is recommended [1989CHI/KNI]. The vaporization enthalpy at $T = 298.15$ K was calculated from vapor pressure data obtained from the Cox equation.

7.9.4. Enthalpy of sublimation

TABLE 53. Sublimation enthalpy of biphenyl

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	298–342	80.9 ± 0.32	320	81.5 ± 0.32	IP	99.98	1989CHI/KNI
2	283–339	83.3 ± 0.92[a]	311	83.7 ± 0.96[b]	PG	99	1989SAS/NGU
3	306–332	80.4 ± 3.2	314	81.0 ± 3.3[b]	GC	na[c]	1975CLA/KNO
4	298	81.8 ± 0.38	298	81.8 ± 0.38	C	99.99	1972MOR
5	288–313	82.5 ± 0.81[a]	301	82.6 ± 0.8[b]	ME	na[c]	1953BRA/CLE

[a] Calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided in the reference.

[b] Sublimation enthalpy adjusted to $T = 298.15$ K using Eq. (3) and an estimated heat capacity for solid biphenyl of 192 J mol^{-1}.

[c] An independent analysis of composition other than a physical property such as melting point is not available.

Recommendation

$\Delta_{\mathrm{sub}} H_{\mathrm{m}}^{\mathrm{o}}$ (298.15 K)	82.1 ± 2.1 kJ mol^{-1}	Recommended value	Entries 1–5

Evaluation

The sublimation enthalpy of biphenyl has been reported many times since the 1950s. The reported values segregate into two sets; one set appears to be centered about a mean of 76.0 kJ mol^{-1} and the other about a mean of 82.0 kJ mol^{-1}. The most recent measurements appear in good agreement with each other and are consistent with the larger of the two values. The mean of the five measurements reported in the table above is 82.1 ± 2.1 kJ mol^{-1} and is the recommended value. Biphenyl has been proposed as a tertiary reference material for sublimation enthalpy measurements [1999SAB/XU].

TABLE 54. Additional sublimation enthalpy values reported for biphenyl since 1950

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})^{\mathrm{a}}$ kJ mol^{-1}	Method	Purity %	Reference
1	298	82.9	298	82.9	CGC-DSC	99	1998CHI/HES,1995HOS
2	313–453	81.8	na	na	GS	99.9	1995NAS/LEN
3	278–298	84.1 ± 0.4	288	83.8 ± 0.1	GS	99	1984BUR/ARM
4	298	77.92 ± 0.28	298	77.92 ± 0.28	C	99+	1979SAB/LAF
5	298	81.75 ± 0.2	298	81.75 ± 0.2	C	99.98	1978MON/ROS
6	273–313	76.0 ± 8.0	293	75.8 ± 8.0	HSA	99	1975CHI
7	298–323	83.6 ± 5.0	310	83.9 ± 5.0	ME	na$^{\mathrm{b}}$	1974RAD/KAT
8	283–293	75.2	308	75.5	ME	na$^{\mathrm{b}}$	1974PRI/POU
9	279–299	75.8	285	75.4	VG	na$^{\mathrm{b}}$	1959AIH
10	288–313	75.1 ± 1.7	298	75.1 ± 1.7	ME	na$^{\mathrm{b}}$	1953SEK/SUZ
11	278–308	72.8 ± 6.0	302	72.9 ± 6.0	ME	na$^{\mathrm{b}}$	1951BRI

[a] Sublimation enthalpy adjusted to $T = 298.15$ K using Eq. (3) and an estimated heat capacity for solid biphenyl of 192 J mol^{-1}.
[b] An independent analysis of composition other than a physical property such as melting point is not available.

7.9.5. Summary

TABLE 55. A summary of experimental and estimated phase change enthalpies for biphenyl

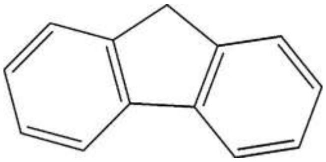
	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K}) + \Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.	18.57 ± 0.01	16.6 ± 0.7	64.9 ± 1.3	82.1 ± 2.1	81.5 ± 1.5
estimated	20.2		59.3		79.5$^{\mathrm{a}}$

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}}) = 59$ J mol^{-1} K^{-1}.

TABLE 56. A summary of recommended enthalpies of sublimation and formation in the condensed and gas phases for biphenyl

$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{cd}, 298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{g}, 298.15\ \mathrm{K})$ kJ mol^{-1}
98.2 ± 2.5	82.1 ± 2.1	180.3 ± 3.3

7.10. Fluorene



Name	Formula	Registry Number	Molecular Weight
Fluorene	$C_{13}H_{10}$	[86-73-7]	166.2185 g mol^{-1}

7.10.1. Enthalpy of formation (solid)

TABLE 57. Standard enthalpies of combustion and formation of fluorene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_rH^o_m$(cr) kJ mol^{-1}	$\Delta_fH^o_m$(cr) kJ mol^{-1}	Reference
1	99.99+	i-SMB	GC, DSC	6	paraffin oil ($CH_{1.94}$)	m	−6635.0 ± 2.2	90.2 ± 2.8	1994RAK/VER
2	99.95	smb	DTA	10	no	m	−6631.3 ± 8.0	86.5 ± 8.0	1987SAB/ANT

Recommendation

$\Delta_fH^o_m$(cr, 298.15 K)	90.2 ± 2.8 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

There are only two bits of data for the enthalpies of combustion and formation of fluorene in the literature and both values fall within their respective uncertainty intervals. The most recent value reported by Rakus *et al.* is suggested [1994RAK/VER].

7.10.2. Enthalpy of fusion

TABLE 58. Fusion enthalpy of fluorene

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H^o_m$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	19.1	387.7	14.80	DSC	99.9	2000LIS/JAM
2	19.46	387	15.2	DSC	99.99	1994RAK/VER
3	19.58 ± 0.06	387.9	15.26 ± 1.4	AC	99.992	1977FIN/MES
4	19.5 ± 0.3	387	15.2 ± 1.4	DSC	EWL[b]	1972WAU/GET
5	19.87	387	15.6	na	na	1996DOM/HEA, 1944EIB

[a] Fusion enthalpies adjusted to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid fluorene of 261.5 and 198.6 J mol^{-1} K^{-1}, respectively.

[b] Recrystallized Eastman White Label.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	19.58 ± 0.06 kJ mol^{-1}	Recommended value	Entry 3
$\Delta_{fus}H^o_m$ (298.15 K)	15.3 ± 1.4 kJ mol^{-1}	Recommended value	Entry 3

Evaluation

The fusion enthalpy measured by Finke *et al.* [1977FIN/MES] using an adiabatic calorimeter is recommended. The fusion enthalpy was adjusted to T=298.15 K as noted above; the uncertainty includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.10.3. Enthalpy of vaporization

TABLE 59. Vaporization enthalpy of fluorene

Entry	T_{Range} K	$\Delta_{\text{vap}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	74.4 ± 2.3	GC	98+	2006HAF/PAR
2	na	na	na	66.9	GC	99	2002LEI/CHA
3	298	72.3 ± 1.1	298	72.3 ± 1.1	CGC	99[a]	1998CHI/HES, 1995HOS[b]
4	383–428	63.3 ± 0.3[c]	398	71.2 ± 1.6[d]	PG	99+	1988SAS/JOS
5	402–568	58.1	419	67.7[d]	na	na	1947STU
6	423–573	56.8 ± 0.2[c]	504	72.9 ± 3.3[d]	I	na	1923MOR/MUR

[a] Not relevant to the measurement; the chromatography generally separates any impurities.
[b] Value recalculated using the recommended vaporization enthalpies of the standards provided by Ruzicka and Majer [1994RUZ/MAJ].
[c] Calculated from the vapor pressures reported over the temperature range indicated by a Clausius-Clapeyron treatment of the data.
[d] Vaporization enthalpies adjusted to $T = 298.15$ K using Eq. (2) and an estimated heat capacity for liquid fluorene of 261.5 J mol^{-1} K^{-}.

Recommendation

$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}$ (298.15 K)	72.1 ± 1.9 kJ mol^{-1}	Suggested value	Entries 3, 4, 6

Evaluation

The suggested value is the average of entries 3, 4, and 6; the uncertainty includes the standard deviation of the mean ($\pm 2\sigma$) and the average uncertainty associated with the temperature adjustment according to Eq. (6).

7.10.4. Enthalpy of sublimation

TABLE 60. Sublimation enthalpy of fluorene

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	298–324	87.1 ± 3.8	311	87.5 ± 3.8[a]	ME	97	2008GOL/SUU
2	289–359	na	324	86.1 ± 0.3	T	na[b]	2004VER
3	298	87.6	298	87.6	CGC-DSC	98[c]	1998CHI/HES, 1995HOS
4	313–453	84.9	na	na	GS	99.9	1995NAS/LEN
5	323–363	84.9 ± 0.4	343	85.1 ± 0.4	GS	99.99	1994RAK/VER
6	303–373	87.0 ± 0.5[d]	338	88.2 ± 0.6[a]	PG	99+	1988SAS/JOS
7	298	80.2 ± 0.2	298	80.2 ± 0.2	C	99	1987SAB/ANT
8	348–388	78.9[e]	363	80.9[a]	na	na	1987STE/MAL
9	306–323	82.8[e]	315	83.3[a]	na	na	1987STE/MAL
10	307–348	83.3	328	84.2[a]	GS	95	1986SAT/INO
11	283–323	88.4 ± 0.6	303	88.6[a]	GS	na	1983SON/ZOL
12	348–387	82.1[e]	368	84.3	IP	99.99	1975OSB/DOU
13	286–300	80.3 ± 0.8	293	80.1 ± 0.8[a]	TE	na	1960BUD
14	306–323	82.8	315	83.3[a]	ME	na	1953BRA/CLE

[a] Sublimation enthalpies adjusted to $T = 298.15$ K using Eq. (3) and an estimated heat capacity for solid fluorene of 198.6 J mol^{-1} K^{-1}.
[b] Although the purity is not stated, Verevkin discussed the presence of approximately 5% impurity very similar in properties to fluorene that could only be removed by 25 recrystallizations.
[c] Not relevant to the measurement; the chromatography generally separates any impurities.
[d] Calculated from the vapor pressures reported over the temperature range indicated by a Clausius-Clapeyron treatment of the data.
[e] Calculated from the Antoine constants.

Recommendation

$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$(298.15 K)	86.5 ± 1.3 kJ mol^{-1}	Suggested value	Entries 1–3, 5, 6, 12

Evaluation

The suggested value is the average of entries 1–3, 5, 6, and 12. The uncertainty represents two standard deviations of the mean. Uncertainties associated with the temperature adjustments are small. No experimental details are provided in 1995NAS/LEN.

7.10.5. Summary

TABLE 61. A summary of experimental and estimated phase change enthalpies for fluorene

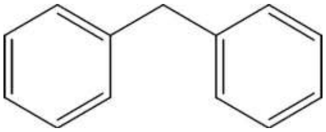
	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)+\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}
expt.	19.58 ± 0.06	15.3 ± 1.4	72.1 ± 1.9	86.5 ± 1.3	87.4 ± 2.4
estimated	19.7		64		83.7[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=50.8\ J\ mol^{-1}\ K^{-1}$.

TABLE 62. A summary of suggested enthalpies of sublimation and formation in the condensed and gas phases for fluorene

$\Delta_fH_m^o(cd, 298.15\ K)$ kJ mol^{-1}	$\Delta_{sub}H_m^o(298.15\ K)$ kJ mol^{-1}	$\Delta_fH_m^o(g, 298.15\ K)$ kJ mol^{-1}
90.2 ± 2.8	86.5 ± 1.3	176.7 ± 3.1

7.11. Diphenylmethane



Name	Formula	Registry Number	Molecular Weight
Diphenylmethane	$C_{13}H_{12}$	[101-81-5]	168.234 38 g mol^{-1}

7.11.1. Enthalpy of formation (liquid)

TABLE 63. Standard enthalpies of combustion and formation of liquid diphenylmethane at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_cH_m^o(l)$ kJ mol^{-1}	$\Delta_fH_m^o(l)$ kJ mol^{-1}	Reference
1	99.98	RMB	Fractional melting	6	oil	m	−6927.7 ± 1.4	97.1 ± 2.2	1995STE/CHI
2	Eastman sample[a]	SMB	mp: 298.3 K	5	na	m	−6923.9 ± 1.3	93.3 ± 2.2	1995STE/CHI, 1950PAR/MOS
3	Eastman sample[b]	SMB	mp: 298.3 K	5	no	m	−6921.4 ± 2.8	90.8 ± 3.2	1995STE/CHI, 1946PAR/WES

[a] Purified by nine fractional crystallizations and utilized immediately after preparation.

[b] Purified by three fractional crystallizations after having stood in a bottle of transparent glass for almost 2 months prior to the combustions and probably deteriorated with time.

Recommendation

$\Delta_fH_m^o$ (l, 298.15 K)	97.1 ± 2.2 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

On the measurement of the energy of combustion of diphenylmethane, a problem arose as to the state (solid or liquid) of the sample within the bomb calorimeter under 3.04 MPa pressure of oxygen at $T=296-297$ K (mp=298.3 K). In this regard, Steel *et al.* [1995STE/CHI] confirmed that the sample is in a liquid state under their experimental conditions. Therefore, the value reported in 1995STE/CHI is suggested.

7.11.2. Enthalpy of formation (solid)

Table 64. Standard enthalpies of combustion and formation of crystalline diphenylmethane at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m$(cd) kJ mol^{-1}	$\Delta_f H^o_m$(cd) kJ mol^{-1}	Reference
1	Eastman sample	SMB	mp: 298.3 K	5	na	m	-6905.7 ± 1.3	75.1 ± 2.2	1995STE/CHI, 1950PAR/MOS
2	99.9	SMB	ea, mp: 298.4 K	na	na	na	-6673.5	-157	1951SER/WIS
3	na	na	na	na	na	na	-6931.2	100.6	2005AFE/LIE, 1951WIS/SER
4	na	SMB	na	5	na	na	-6929.5 ± 0.8^a	98.9 ± 1.9	1995STE/CHI, 1946COO/MUL
5	na	SMB	na	na	na	na	-6945.0	114.4	2005AFE/LIE,1906SCH

[a] The authors report the value of the enthalpy of formation in the crystalline state without any confirmation of the state of the sample under their experimental conditions. However, the value determined is in good agreement with the values reported by Steele *et al.* [1995STE/CHI] for the liquid sample. Therefore, the sample is probably in the liquid state under the experimental conditions.

Recommendation

$\Delta_f H^o_m$(cr, 298.15 K)	75.1 ± 2.2 kJ mol^{-1}	Suggested value	Entry 1

7.11.3. Enthalpy of fusion

Table 65. Fusion enthalpy of diphenylmethane

Entry	$\Delta_{fus} H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus} H^o_m$(298 K) kJ mol^{-1}	Method	Purity %	Reference
1	19.01 ± 0.01	298.3^a	19.01 ± 0.01	AC	99.98	2005CHI/STE, 1995STE/CHI
2	19.25	298	19.25	DSC	99	1986CHI/ANN
3	18.8	299	18.8	na	na	1938WOL/WEG
4	18.58	298.4	18.58	na	na	1931PAR/HUF

[a] Triple point.

Recommendation

$\Delta_{fus} H_m$ (T_{fus})	19.01 ± 0.01 kJ mol^{-1}	Recommended value	Entry 1
$\Delta_{fus} H^o_m$(298.15 K)	19.01 ± 0.01 kJ mol^{-1}	Recommended value	Entry 1

7.11.4. Enthalpy of vaporization

Table 66. Vaporization enthalpy of diphenylmethane

Entry	T_{Range} K	$\Delta_{vap} H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap} H^o_m$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	64.71 ± 0.3	GC	na	2006HAF/PAR
2	329–588	62.52 ± 0.12	360	67.6 ± 0.16	IP	99.98	2005CHI/STE
3	303–343	66.36 ± 0.5	323	67.9 ± 0.8	GS	99.99	1999VER
4	na	na	na	63.11	GC	na	1996GOV/RUT
5	353–433	60.2^a	393	68.1^b	GS	99.8+	1990SOH/OKA
6	304–333	66.8 ± 1.5^c	319	68.5 ± 1.6^b	PG	99	1989SAS/NGU
7	424–521	56.83 ± 0.8	440	68.7 ± 3.5	DM	99	1980WIE/KOB
8	298	67.5 ± 0.1	298	67.5 ± 0.1	C	na	1972MOR

[a] Calculated from the Antoine constants.

[b] Vaporization enthalpies adjusted to T=298.15 K using Eq. (2) and an estimated heat capacity for liquid diphenylmethane of 280.5 J mol^{-1} K^{-1}.

[c] Calculated from the experimental vapor pressures reported over the temperature range indicated by a Clausius-Clapeyron treatment of the data.

Recommendation

$\Delta_{vap} H^o_m$(298.15 K)	67.9 ± 0.4 kJ mol^{-1}	Recommended value	Entries 2, 3, 5, 6, 8

Evaluation

The recommended value is the average of all entries except 1, 4, and 7; the latter has a large adjustment for temperature; the uncertainty is two standard deviations of the mean ($\pm 2\sigma$).

7.11.5. Enthalpy of sublimation

TABLE 67. Sublimation enthalpy of diphenylmethane

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	270–298	87.35 ± 0.1^{a}	284	86.88 ± 0.2^{b}	IP	99.98	2005CHI/STE
2	273–295	88.46 ± 0.82	284	87.6 ± 0.8	GS	99.99	1999VER
3	274–298	71.6 ± 1.1	286	71.2 ± 1.1^{b}	PG	99	1989SAS/NGU
4	273–295	83.3 ± 8.4	285	82.9 ± 8.4^{b}	HSA	99	1986CHI/ANN
5	278–298	82.46^{d}	288	81.7^{a}	VG	na	1959AIH
6	278–300	64.0 ± 2.9	289	63.2 ± 2.9^{a}	ME	na	1951BRI
7	299	72.0 ± 1.6	299	72.0 ± 1.6^{a}	QF	na	1938WOL/WEG

[a] Calculated from the vapor pressure equation given.
[b] Sublimation enthalpy adjusted to $T = 298.15$ K using Eq. (3) and an estimated heat capacity for solid diphenylmethane of 218.9 J mol^{-1} K^{-1}.
[c] Calculated from the experimental vapor pressures reported over the temperature range indicated by a Clausius-Clapeyron treatment of the data.
[d] This value is calculated from the equation listed below the vapor pressure data given in the paper; calculation of the sublimation enthalpy using the vapor pressure data results in a sublimation enthalpy of 74.19 ± 2.8 kJ mol^{-1}.

Recommendation

$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$ (298.15 K)	87.2 ± 0.7 kJ mol^{-1}	Recommended value	Entries 1 and 2

Evaluation

The recommended value is the average of the first two entries. The uncertainty is two standard deviations of the mean.

7.11.6. Summary

TABLE 68. A summary of experimental and estimated phase change enthalpies for diphenylmethane

	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}$(298 K) kJ mol^{-1}	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}$(298 K) kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$(298 K) kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}$(298 K)+ $\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}$(298 K) kJ mol^{-1}
expt.	19.01 ± 0.01	19.01 ± 0.01	67.9 ± 0.4	87.2 ± 0.7	86.9 ± 0.4
estimated	18.5		59.3		77.8^{a}

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\text{tpce}}S(T_{\text{fus}}) = 61.9$ J mol^{-1} K^{-1}.

TABLE 69. A summary of suggested enthalpies of vaporization, sublimation, and formation in the condensed and gas phases for diphenylmethane

Phase	$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}$(298.15 K) kJ mol^{-1}	$\Delta_{\text{sub/vap}}H^{\text{o}}_{\text{m}}$(298.15 K) kJ mol^{-1}	$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}$(g, 298.15 K) kJ mol^{-1}
Liquid	97.1 ± 2.2	67.9 ± 0.4	165.0 ± 2.2
Solid	75.1 ± 2.2	87.2 ± 0.7	162.3 ± 2.3

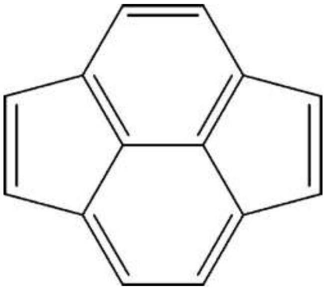
Recommendation

$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}$(g, 298.15 K)	163.7 ± 2.3 kJ mol^{-1}	Suggested value

Evaluation

The suggested value has been calculated as the average of the results obtained for liquid and solid samples.

7.12. Pyracyclene



Name	Formula	Registry Number	Molecular Weight
Pyracyclene	$C_{14}H_8$	[187-78-0]	176.213 32 g mol^{-1}

7.12.1. Enthalpy of formation (solid)

TABLE 70. Standard enthalpies of combustion and formation of pyracyclene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m$(cr) kJ mol^{-1}	$\Delta_f H^o_m$(cr) kJ mol^{-1}	Reference
1	na	smb	na	6	n-hexadecane	m	-6979.1 ± 3.0	326.6 ± 3.6	2002DIO/KIY
2	Sublimed. No impurities detected	smb	^{1}H-NMR, UV	5	n-hexadecane	m	-6976.6 ± 3.1	324.1 ± 3.6	1996DIO/PER

Recommendation

$\Delta_f H^o_m$(cr, 298.15 K)	325.4 ± 3.6 J mol^{-1}	Suggested value	Entries 1 and 2

Evaluation

The values reported for the enthalpy of formation in the condensed state of pyracyclene are within their respective uncertainty intervals. Thus, the suggested value is the mean of both sets of data.

7.12.2. Enthalpy of fusion

Not available.

7.12.3. Enthalpy of vaporization

Not available.

7.12.4. Enthalpy of sublimation

TABLE 71. Sublimation enthalpy of pyracyclene

Entry	T_{Range} K	$\Delta_{\text{sub}} H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}} H^o_m$(298.15 K) kJ mol−1	Method	Purity %	Reference
1	342	82.0	342	83.2	DC	na	2002DIO/KIY

Recommendation

$\Delta_{\text{sub}} H^o_m$(298.15 K)	83.2 kJ mol^{-1}	Available value	Entry 1

7.12.5. Summary

TABLE 72. A summary of experimental and estimated phase change enthalpies for pyracyclene

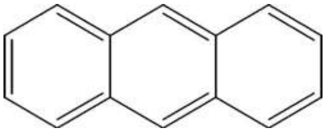
	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\text{ K})+\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}
expt.				83.2	
estimated[a]			68.7		

[a] compound decomposes without melting.

TABLE 73. A summary of available enthalpies of sublimation and formation in the condensed and gas phases for pyracyclene

$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}(\text{cr},298.15\text{ K})$ kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$ kJ mol^{-1}	$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}(\text{g},298.15\text{ K})$ kJ mol^{-1}
325.4 ± 3.6	83.2	408.6

7.13. Anthracene



Name	Formula	Registry Number	Molecular Weight
Anthracene	$C_{14}H_{10}$	[120-12-7]	178.2292 g mol^{-1}

7.13.1. Enthalpy of formation (solid)

TABLE 74. Standard enthalpies of combustion and formation of anthracene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_{\text{r}}H^{\text{o}}_{\text{m}}(\text{cr}))$ kJ mol^{-1}	$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}(\text{cr})$ kJ mol^{-1}	Reference
1	>99.95	smb	GC	9	n-hexadecane	m	−7062.7 ± 2.1	124.4 ± 2.8	2007RIB/PIL
2	Zrm	i-smb	DSC, mp[a]	5	no	m	−7065.0 ± 1.1	126.5 ± 2.1	2001NAG
3	na	i-rmb	mp[b]	3	no	m	−7063.7 ± 5.3	125.4 ± 5.6	1983MET/KUO
4	99.95, Zrm	i-SMB	Tfmp	4	no	CO_2	−7067.2 ± 1.7	128.9 ± 2.5	1966COL/PIL
5	Zrm	i-smb	mp[c]	6	no	m	−7054.5 ± 4.3	116.2 ± 4.7	1963MAC/OHA
6	na	i-SMB	na	5	no	m	−7067.1 ± 4.2	128.8 ± 4.6	1952BEN/FAR
7	na	i-SMB	mp[d]	4	no	m	−7069.4 ± 1.6	131.1 ± 2.4	1951MAG/HAR
8	0.005% ash	i-SMB	na	5	no	m	−7045.5 ± 2.8	107.2 ± 3.4	1946PAR/WES
9	na	i-SMB	na	6	no	m	−7049.3 ± 2.4	111.0 ± 3.0	1939RIC/PAR
10	na	i-SMB	na	10	no	m	−7071.3 ± 1.5	133.0 ± 2.4	1935FRI/WAL
11	na	i-SMB	na	5	no	m	−7053.9 ± 7.1	115.6 ± 7.3	1970COX/PIL, 1932MIL/ROS
12	na	i-SMB	na	4	no	m	−7056.9 ± 1.3	118.6 ± 2.3	1970COX/PIL, 1931BUR
13	na	i-SMB	na	4	no	m	−7057.3 ± 1.3	119.0 ± 2.3	1931BEC

[a] mp=488.95 K.
[b] mp=488 K.
[c] mp=489.65 K.
[d] mp=489–490 K.

Recommendation

$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}(\text{cr},298.15\text{ K})$	127.5 ± 2.6 kJ mol^{-1}	Recommended value	Entries 2–4

Evaluation

The enthalpies of combustion and formation for anthracene have been determined many times. The recommended value is the weighted average from the results of entries 2–4.

7.13.2. Enthalpy of fusion

TABLE 75. Fusion enthalpy of anthracene

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H_m^o(298\ K)$[a] kJ mol^{-1}	Method	Purity %	Reference
1	29.84 ± 0.9	492	19.94 ± 3.3	DSC	99.95	2003ROJ/ORO
2	28.8	489.4	19.03	DSC	99.89	2000LIS/JAM
3	29.0 ± 0.8	490.6	19.2 ± 3.2	DSC	zr[b]	1980RAD/RAD
4	28.8 ± 2.2	492.7	18.9 ± 3.2	DSC	Puriss[c]	1973CAS/VEC
5	29.0 ± 0.6	490.2	19.2 ± 3.0	DSC	vs[d]	1972WAU/GET
6	29.4 ± 0.1	488.9	19.7 ± 3.2	AC	99.99+	1970GOU/GIR
7	28.8	490	19.0 ± 3.0	na	na	1950UEB/ORT
8	28.83	489.7	19.04	na	na	1931PAR/HUF
9	28.9 ± 0.2	489.7	19.1 ± 3.2	C	na	1917HIL/DUS

[a] Fusion enthalpies adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid anthracene of 279.2 and 209 J mol^{-1} K^{-1}, respectively.

[b] Zone refined.

[c] Fluka AG, Buchs, Switzerland.

[d] Mallinckrodt anthracene (mp: 215–217) vacuum sublimed (three times).

Recommendation

$\Delta_{fus}H_m(T_{fus})$	29.4 ± 0.1 kJ mol^{-1}	Recommended value	1996DOM/HEA
$\Delta_{fus}H_m^o(298.15\ K)$	19.7 ± 3.2 kJ mol^{-1}	Recommended value	Entry 6

Evaluation

The fusion enthalpy of anthracene has been reported several times. Domalski and Hearing recommended a value of 29.4 ± 0.1 kJ mol^{-1} [1996DOM/HEA] measured by adiabatic calorimetry which is also our recommendation. The average fusion enthalpy at the melting temperature of all nine entries is 29.04 ± 0.24 kJ mol^{-1}. The fusion enthalpy of entry 6 was adjusted to 298.15 K as noted above. An average value of all nine values results in a mean value of 19.3 ± 0.23 kJ mol^{-1} at $T=298.15$ K. The uncertainty in the recommended value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.13.3. Enthalpy of vaporization

TABLE 76. Vaporization enthalpy of anthracene

Entry	T_{Range} K	$\Delta_{vap}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H_m^o(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	79.50	GC	na	2006HAF/PAR
2	498.2	66.68 ± 0.8	498.2	83.30 ± 3.3[a]	DSC	99.95	2003ROJ/ORO
3	na	na	na	72.4	GC	99	2002LEI/CHA
4	298	79.8 ± 1.2	298	79.8 ± 1.2	CGC[b]	99+[c]	1998CHI/HES, 1995HOS
5	504–615	58.59[d]	519	77.0[a]	na	na[e]	1987STE/MAL
6	500	62.1 ± 4.0	500	80.5 ± 7.6[a]	na	na[e]	1979KUD/KUD, 1971WIL/ZWO
7	496–555	59.2 ± 0.2[f]	526	78.2 ± 3.6[a]	I	na[e]	1923MOR/MUR
8	500–537	59.4 ± 2.2[f]	519	77.8 ± 4.2[a]	I	na[e]	1922NEL/SEN

[a] Vaporization enthalpy adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity for liquid anthracene of 279.2 J mol^{-1} K^{-1}.

[b] Correlation-gas chromatography.

[c] Not relevant to the measurement; the chromatography generally separates any impurities.

[d] Calculated from the Antoine constants at $T=519$ K.

[e] An independent analysis of composition other than a physical property such as melting point is not available.

[f] Calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided in the reference.

Recommendation

$\Delta_{vap}H^o_m(298.15\ K)$	79.9 ± 4.0 kJ mol^{-1}	Suggested value	Entries 1, 2, 4, 6–8

Evaluation

The suggested vaporization enthalpy is the average of all values but the values cited in the third and fifth entries, which contain no other experimental information. This value is suggested because of the large temperature adjustment needed. The uncertainty was calculated by combining two standards deviations of the mean with an average uncertainty associated with the temperature adjustment according to Eq. (6).

7.13.4. Enthalpy of sublimation

TABLE 77. Sublimation enthalpy of anthracene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	288–323	98.5 ± 3.3	306	98.8 ± 3.3[a]	ME	99	2008GOL/SUU
2	340–360	98.8 ± 0.4	350	100.2 ± 0.4	ME	99.99	2006RIB/MON
3	na	na	453	100.8 ± 1.7	DC	99+	2004SAN/SCH
4	318–363	100.0 ± 2.8	341	101.0 ± 5.6[a]	ME	99+	1998OJA/SUU
5	298	100.8 ± 3.4	298	100.8 ± 3.4	CGC-DSC	99+	1998CHI/HES, 1995HOS
6	313–363	102.6 ± 2.6	338	103.9 ± 2.7[a]	GS	99.9	1986HAN/ECK
7	337–361	100.6 ± 2.0	349	104.5 ± 3.0	TE, ME	zrm[b]	1980DEK
8	353–432	101.04 ± 0.92	393	104.1 ± 1.4[a]	ME	sg[c]	1973MAL/GIG
9	353–432	99.7 ± 1.5	393	102.7 ± 1.8[a]	C	sg[c]	1973MAL/GIG
10	342–359	98.5	351	100.2	ME	na[d]	1964KEL/RIC
11	303–373	103.4	338	104.7[a]	ME	na[d]	1958HOY/PEP
12	378–398	100.8 ± 0.6[e]	388	103.7 ± 2.02[a]	MM	na[d]	1973MAL/GIG, 1958KLO
13	339–354	101.6 ± 4.1	347	103.2 ± 4.4[a]	ME	na[d]	1953BRA/CLE

[a] Sublimation enthalpy adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity of 209 J mol^{-1} K^{-1} for the solid.
[b] Zone refined material.
[c] Scintillation grade (Merck).
[d] An independent analysis of composition other than a physical property such as melting point is not available.
[e] The uncertainty evaluated from the data given.

Recommendation

$\Delta_{sub}H^o_m(298.15\ K)$	101.9 ± 1.3 kJ mol^{-1}	Recommended value	Entries 1–9

Evaluation

Anthracene has been recommended as a standard for sublimation enthalpy measurements. A value of 103.36 ± 2.7 kJ mol^{-1} was previously recommended [1999SAB/XU]. This value was based on the measurements recorded in entries 6/13. Several new reports are now available since this recommendation. While the new values fall within the specified experimental uncertainties, the consistency in these values suggests that the recommended value for anthracene should be revisited. An argument against modifying the value at this time is that two of these reports (entries 2 and 3) use anthracene as a test case for the development of a new apparatus. However in both cases, additional reference materials are used for this purpose. The new recommended value is based on the mean of the first nine entries for which some assessment of purity is provided. The uncertainty represents two standard deviations of the mean.

TABLE 78. Additional sublimation enthalpy values reported for anthracene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
14	423–488	94.5	456	99.6[a]	T	na	1999EMM/PIC
15	313–453	99.7	na	na	GS	99	1995NAS/LEN
16	354–399	94.6	376	97.1[a]	GS	99.9	1983BEN/BIE
17	283–323	91.8 ± 1.8	303	92.0 ± 1.8	GS	na[b]	1983SON/ZOL
18	na	97.4 ± 2.2	na	na	DSC	99.98	1981BRO/MCE

TABLE 78. Additional sublimation enthalpy values reported for anthracene—Continued

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\circ}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
19	na	97.8 ± 0.2	na	na	HSA	na	1980DYG/STE
20	358–393	94.8	376	97.3[a]	GS	99+	1979MAC/PRA
21	363–448	98.8 ± 0.8	na	na	HSA	na[b]	1977DYG/STE
22	329–373	97.3	351	99.0[a]	ME	na[b]	1976TAY/CRO
23	421	96.0 ± 2	421	97.1 ± 2	DC	na[b]	1975ADE/LAL
24	290–358	84.2 ± 5.4	324	84.9 ± 5.5[a]	ME	na[b]	1972WIE
25	420–540	126 ± 4.0	480	131.8 ± 4.4[a]	DSC	na	1971BEE/LIN
26	396–421	97.5 ± 4	408	101.0 ± 4.6[a]	HSA	na[b]	1953STE
27	352–376	92.5 ± 4.2[c]	364	94.1 ± 4.2[a]	ME	na[b]	1952INO/SHI
28	378–398	97.3 ± 4.4	388	100.2 ± 4.4[a]	RG	na[b]	1949SEA/HOP
29	353	93.3 ± 8.4	353	95.1 ± 8.4[a]	na	na[b]	1938WOL/WEG

[a] Sublimation enthalpy adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity of 209 J mol^{-1} K^{-1} for the solid.
[b] An independent analysis of composition other than a physical property such as melting point is not available.
[c] Two “polymorphic” forms of anthracene are described in these work; these data refer to form II.

7.13.5. Summary

TABLE 79. A summary of experimental and estimated phase change enthalpies for anthracene

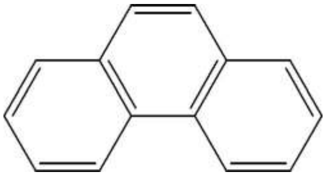
	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol – 1	$\Delta_{\mathrm{fus}}H^{\circ}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol – 1	$\Delta_{\mathrm{vap}}H^{\circ}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol – 1	$\Delta_{\mathrm{sub}}H^{\circ}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol – 1	$\Delta_{\mathrm{fus}}H^{\circ}_{\mathrm{m}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H^{\circ}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol – 1
expt.	29.4 ± 0.1	19.7 ± 3.2	79.9 ± 4.0	101.9 ± 1.3	99.6 ± 5.1
estimated	21.5		68.7		90.2[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=44$ J mol^{-1} K^{-1}.

TABLE 80. A summary of recommended enthalpies of sublimation and formation in the condensed and gas phases for anthracene

$\Delta_{\mathrm{f}}H^{\circ}_{\mathrm{m}}(\mathrm{cr},298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\circ}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H^{\circ}_{\mathrm{m}}(\mathrm{g},298.15\ \mathrm{K})$ kJ mol^{-1}
127.5 ± 2.6	101.9 ± 1.3	229.4 ± 2.9

7.14. Phenanthrene



Name	Formula	Registry Number	Molecular Weight
Phenanthrene	$C_{14}H_{10}$	[85-01-8]	178.2292 g mol^{-1}

7.14.1. Enthalpy of formation (solid)

TABLE 81. Standard enthalpies of combustion and formation of phenanthrene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num of exp.	Aux. Subs.	Amount Reactn.	$\Delta_{\mathrm{r}}H^{\circ}_{\mathrm{m}}(\mathrm{cr})$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H^{\circ}_{\mathrm{m}}(\mathrm{cr})$ kJ mol^{-1}	Reference
1	99.99, Zrm	i-smb	DSC	4	no	m	−7048.6 ± 0.9	110.4 ± 2.0	2002NAG
2	99.987	i-SMB	cfm	7	no	CO_2	−7047.9 ± 1.5	109.6 ± 2.4	1990STE/CHI

TABLE 81. Standard enthalpies of combustion and formation of phenanthrene at $T=298.15$ K—Continued

Entry	Purity %	Method	Charact.	Num of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H_m^o$(cr) kJ mol^{-1}	$\Delta_f H_m^o$(cr) kJ mol^{-1}	Reference
3	99.97, Zrm	i-SMB	Tfmp	5	no	CO_2	-7054.5 ± 1.3	116.1 ± 2.3	1966COL/PIL
						m	-7049.3 ± 1.3	111.0 ± 2.3	2003NAG/NAK, 1966COL/PIL
4	99.95	i-SMB	na	3	no	m	-7052.2 ± 2.9	113.9 ± 3.4	1952BEN/FAR
5	na	i-SMB	mp:99.5–100 °C	5	no	m	-7049.3 ± 1.4	111.0 ± 2.3	1951MAG/HAR
6	0.007% ash	i-SMB	na	4	no	m	-7012.6 ± 2.5	74.3 ± 3.1	1939RIC/PAR
7	na	i-SMB	na	6	no	m	-7052.1 ± 1.3	113.8 ± 2.3	1935FRI/WAL
8	na	i-SMB	na	5	no	m	-7008.6 ± 7.1	70.3 ± 7.3	1970COX/PIL, 1932MIL/ROS

Recommendation

$\Delta_f H_m^o$(cr, 298.15 K)	110.1 ± 2.2 kJ mol^{-1}	Recommended value	Entries 1 and 2

Evaluation

The enthalpy of formation in the condensed state of phenanthrene has been reported several times. The selected value has been calculated as a weighted average from Nagano [2002NAG] and Steele *et al.* [1990STE/CHI]. The recommended value predicts a more accurate equilibrium constant for the hydrogenation of phenanthrene [2003NAG/NAK, 1990STE/CHI] than using the value of Coleman and Pilcher [1966COL/PIL]. In addition, the strain energy of phenanthrene obtained using the recommended value agrees well with estimation from semiempirical calculations and from the basicity in a solution of HF [2003NAG/NAK].

7.14.2. Enthalpy of fusion

TABLE 82. Fusion enthalpy of phenanthrene

Entry	$\Delta_{trans} H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus} H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{tpce} H_m^o$(298 K) kJ mol^{-1}	Method	Purity %	Reference
1	0.85 ± 0.07	345.2	16.57 ± 0.02	367.6	13.87 ± 1.2^a	DSC	99.94	2003ROJ/ORO
2	na	na	16.2	372.9	13.2^a	DSC	99.86	2000LIS/JAM
3	na	na	15.7 ± 0.2	373.8	11.8 ± 3.9^b	DTA	99.74	1992SAB/ELW
4	1.0	332.2	na	na	na	DSC	na	1988PET/TSY
5	na	na	18.63	373	14.8^b	na	na	1987RAI/SIN
6	0.22	347.5	16.46 ± 0.04	372.4	12.89 ± 1.25^a	AC	99.9+	1977FIN/MES
7	1.3	338	16.7 ± 0.6	371.3	14.3 ± 1.2^a	DSC	Purum^c	1973CAS/VEC
8	na	na	16.28	na	na	DSC	na	1972WAU/GET
9	na	na	18.1 ± 0.7	373.2	14.3 ± 1.3^b	C	mp^d	1964RAS/BAS
10	2.6	342	18.62	373	17.4^a	na	na	1950UEB/ORT
11	na	na	18.62	369.5	15.0^b	na	na	1931PAR/HUF

[a] $\Delta_{tpce} H_m(T_{fus})$ adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid phenanthrene of 279.2 and 209 J mol^{-1} K^{-1}, respectively.

[b] $\Delta_{fus} H_m^o$ adjusted to $T=298.15$ K as in footnote a.

[c] Fluka, AG, Buchs, Switzerland.

[d] Characterized by melting point, 353.5 K; E. Merck; extra pure.

Recommendation

$\Delta_{fus} H_m(T_{fus})$	16.46 ± 0.04 kJ mol^{-1}	Recommended value	Entry 7
$\Delta_{tpce} H_m^o$(298.15 K)	12.9 ± 1.3 kJ mol^{-1}	Recommended value	Entry 7

Evaluation

The fusion enthalpy of phenanthrene has been reported several times. The recommended value is that of Finke *et al.* [1977FIN/MES]. A similar recommendation has been made by Domalski and Hearing [1996DOM/HEA]. This fusion enthalpy was adjusted to $T=298.15$ K, combined with the observed enthalpy of transition and reported as the recommended value for $\Delta_{tpce} H_m^o$(298.15 K); the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.14.3. Enthalpy of vaporization

TABLE 83. Vaporization enthalpy of phenanthrene

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	79.0 ± 2.4	GC	98+	2006HAF/PAR
2	388	68.9 ± 1.6	388	$76.4 \pm 2.2^{\mathrm{a}}$	DSC	99.94	2003ROJ/ORO
3	na	na	na	72.2	GC	99	2002LEI/CHA
4	372.4	71.1	372.4	77.9^{a}	PG	99.5	1998RUZ/MOK
5	298	78.7 ± 1.1	298	78.7 ± 1.1	CGC	99	1998CHI/HES, 1995HOS
6	372–463	68.4 ± 0.5	418	$78.4 \pm 2.0^{\mathrm{a}}$	na	97	1995MOK/GUE
7	372.4	71.2	372.4	77.4			1979KUD/KUD
8	373–423	$68.95 \pm 0.4^{\mathrm{b}}$	398	77.3 ± 1.6	IP	99.99	1977FIN/MES, 1975OSB/DOU
9	507–545	$60.83 \pm 0.3^{\mathrm{b}}$	526	79.8 ± 3.6	I	na$^{\mathrm{c}}$	1923MOR/MUR
10	505–538	$61.76 \pm 1.5^{\mathrm{b}}$	522	80.4 ± 3.9	I	na$^{\mathrm{c}}$	1922NEL/SEN

[a] Vaporization enthalpy adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity for liquid phenanthrene of 279.2 J mol^{-1} K^{-1}.

[b] Calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided in the reference.

[c] An independent analysis of composition is not available.

Recommendation

$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(372\ \mathrm{K})$	71.7 kJ mol^{-1}	Recommended value	Entry 4
$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	78.3 ± 1.8 kJ mol^{-1}	Recommended value	Entries 1, 2, 4–10

Evaluation

Entry 4 has been recommended as the vaporization enthalpy at the triple point, $T=372.4$ K. Adjusting to $T=298.15$ results in a value of 77.9 kJ mol^{-1}. No uncertainty is reported with this value. The value recommended at $T=298.15$ K is the mean of all values except entry 3. The uncertainty in the recommended value represents two standard deviations of the mean (± 0.8 kJ mol^{-1}) and the average ($\pm 2\sigma$) uncertainty is associated with the temperature adjustment (± 1.6 kJ mol^{-1}).

7.14.4. Enthalpy of sublimation

TABLE 84. Sublimation enthalpy of phenanthrene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	313–333	91.6	323	92.5 ± 0.4	ME	99.8+	2006RIB/MON
2	372.4	90.34	372.4	92.12	PG	99.5	1998RUZ/MOK
3	303–333	95.0 ± 4.4	318	$95.6 \pm 8.8^{\mathrm{a}}$	ME	99	1998OJA/SUU
4	298	91.6 ± 1.8	298	91.6 ± 1.8	CGC-DSC	99	1998CHI/HES, 1995HOS
5	350	87.24 ± 2.2	350	$91.1 \pm 3.4^{\mathrm{a,c}}$	DSC	99.5+	1988TOR/BAR
6	315–335	90.5 ± 2.0	325	92.5 ± 4.0	TE, ME	na$^{\mathrm{a}}$	1980DEK
7	298	90.88 ± 0.8	298	90.88 ± 0.8	C	99.97	1972MOR

[a] Sublimation enthalpy adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for crystalline phenanthrene of 209 J mol^{-1} K^{-1}.

[b] Known to contain less than 0.1 mass % anthracene.

[c] Included a phase transition of 0.2 kJ mol^{-1}.

Recommendation

$\Delta_{\rm sub}H_{\rm m}^{\rm o}(372.4\ {\rm K})$	90.34 kJ mol^{-1}	Recommended value	Entry 2
$\Delta_{\rm sub}H_{\rm m}^{\rm o}(298.15\ {\rm K})$	92.1 ± 0.6 kJ mol^{-1}	Recommended value	Entry 2

Evaluation

Phenanthrene has previously been recommended as a tertiary standard for sublimation enthalpy measurements [1999SAB/XU] on the basis of entries 5–7. A value of 91.3 ± 2.7 kJ mol^{-1} was previously suggested. Additional measurements have been reported since this recommendation and reviewed in light of the new recommendation [1998RUZ/MOK]. The new value is the value recommended by Ruzicka *et al.* and is within the uncertainty limits of the previous measurements. Omitting the third entry, the average of all six measurements is 91.8 ± 0.6 kJ mol^{-1}. Since no uncertainty was assigned to this recommended value, an uncertainty is assigned based on two standard deviations of the mean of all six entries.

TABLE 85. Additional sublimation enthalpy values reported for phenanthrene

Entry	$T_{\rm Range}$ K	$\Delta_{\rm sub}H_{\rm m}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\rm sub}H_{\rm m}^{\rm o}(298.15\ {\rm K})^{\rm a}$ kJ mol^{-1}	Method	Reference
8	313–453	88.9	na	na	GS	1995NAS/LEN
9	283–323	95.0 ± 1.2	303	95.1 ± 1.2	GS	1983SON/ZOL
10	317–362	80.4 ± 2.7	340	81.8 ± 1.4	TE	1983FER/IMP
11	325–363	$87.19 \pm 1.9^{\rm b}$	344	88.7 ± 2.0	GS	1979MAC/PRA
12	297–315	84.1 ± 5.0	306	84.4 ± 5.0	TE	1960BUD
13	273–333	95.9	303	96.1	na	1958HOY/PEP
14	310–322	86.6	316	87.2	ME	1953BRA/CLE
15	315	90.7 ± 2.4	315	91.2 ± 2.4	ME	1952INO/SHI
16	313	84.1 ± 1.6	313	84.6 ± 1.6	na	1938WOL/WEG

[a] Sublimation enthalpy adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity of 209 J mol^{-1} K^{-1} for the solid.

[b] Calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided in the reference.

7.14.5. Summary

TABLE 86. A summary of experimental and estimated phase change enthalpies for phenanthrene

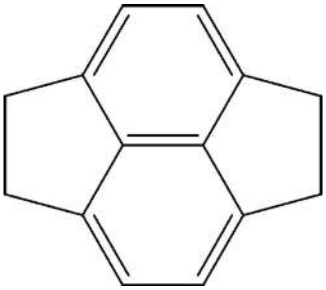
	$\Delta_{\rm fus}H_{\rm m}(T_{\rm fus})$ kJ mol^{-1}	$\Delta_{\rm tpce}H_{\rm m}^{\rm o}(298\ {\rm K})$ kJ mol^{-1}	$\Delta_{\rm vap}H_{\rm m}^{\rm o}(298\ {\rm K})$ kJ mol^{-1}	$\Delta_{\rm sub}H_{\rm m}^{\rm o}(298\ {\rm K})$ kJ mol^{-1}	$\Delta_{\rm fus}H_{\rm m}^{\rm o}(298\ {\rm K})+\Delta_{\rm vap}H_{\rm m}^{\rm o}(298\ {\rm K})$ kJ mol^{-1}
expt.	16.46 ± 0.04	12.9 ± 1.3	78.3 ± 1.8	92.1 ± 0.6	91.2 ± 2.2
estimated	16.4		68.7		$85.1^{\rm a}$

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\rm tpce}S(T_{\rm fus})=44$ J mol^{-1} K^{-1}.

TABLE 87. A summary of recommended enthalpies of sublimation and formation in the condensed and gas phases for phenanthrene

$\Delta_{\rm f}H_{\rm m}^{\rm o}({\rm cr},298.15\ {\rm K})$ kJ mol^{-1}	$\Delta_{\rm sub}H_{\rm m}^{\rm o}(298.15\ {\rm K})$ kJ mol^{-1}	$\Delta_{\rm f}H_{\rm m}^{\rm o}({\rm g},298.15\ {\rm K})$ kJ mol^{-1}
110.1 ± 2.2	92.1 ± 0.6	202.2 ± 2.3

7.15. Pyracene



Name	Formula	Registry Number	Molecular Weight
Pyracene	$C_{14}H_{12}$	[567-79-3]	180.245 08 g mol^{-1}

7.15.1. Enthalpy of formation (solid)

TABLE 88. Standard enthalpies of combustion and formation of pyracene at T=298.15 K

	Purity						$\Delta_r H^o_m$(cr)	$\Delta_f H^o_m$(cr)	
Entry	%	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	kJ mol^{-1}	kJ mol^{-1}	Reference
1	>99.5 (GC)	smb	H-NMR, ea, UV, mp[a]	5	HDN[b]	m	−7308.8 ± 3.7	84.7 ± 4.1	2002DIO/KIY

[a] mp: 489.7–490.7 K.
[b] n-hexadecane.

Recommendation

$\Delta_f H^o_m$(cr, 298.15 K)	84.7 ± 4.1 kJ mol^{-1}	Available value	Entry 1

7.15.2. Enthalpy of fusion

Not available; T_{fus}=490 K.

7.15.3. Enthalpy of vaporization

Not available.

7.15.4. Enthalpy of sublimation

TABLE 89. Sublimation enthalpy of pyracene

	T_{Range}	$\Delta_{sub}H_m(\bar{T})$	$\bar{T}$	$\Delta_{sub}H^o_m$(298.15 K)		Purity	
Entry	K	kJ mol^{-1}	K	kJ mol^{-1}	Method	%	Reference
1	324–354	88.8 ± 3.0	339	89.6 ± 3.3	ME	99.5	2002DIO/KIY

Recommendation

$\Delta_{sub}H^o_m$(298.15 K)	89.6 ± 3.3 kJ mol^{-1}	Available value	Entry 1

7.15.5. Summary

TABLE 90. A summary of experimental and estimated phase change enthalpies for pyracene

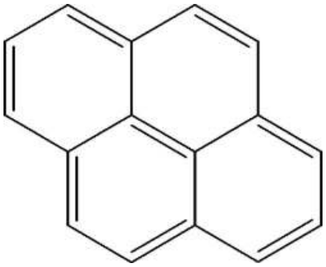
	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$
	$\mathrm{kJ\ mol^{-1}}$	$\mathrm{kJ\ mol^{-1}}$	$\mathrm{kJ\ mol^{-1}}$	$\mathrm{kJ\ mol^{-1}}$	$\mathrm{kJ\ mol^{-1}}$
expt.				89.6 ± 3.3	
estimated	18.3		68.7		87[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=37.4\ \mathrm{J\ mol^{-1}\ K^{-1}}$.

TABLE 91. A summary of available enthalpies of sublimation and formation in the condensed and gas phases for pyracene

$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}(\mathrm{cr},\ 298.15\ \mathrm{K})$	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}(\mathrm{g},298.15\ \mathrm{K})$
$\mathrm{kJ\ mol^{-1}}$	$\mathrm{kJ\ mol^{-1}}$	$\mathrm{kJ\ mol^{-1}}$
84.7 ± 4.1	89.6 ± 3.3	174.3 ± 5.3

7.16. Pyrene



Name	Formula	Registry Number	Molecular Weight
Pyrene	$C_{16}H_{10}$	[129-00-0]	$202.2506\ \mathrm{g\ mol^{-1}}$

7.16.1. Enthalpy of formation (solid)

TABLE 92. Standard enthalpies of combustion and formation of pyrene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_{\mathrm{r}}H^{\mathrm{o}}_{\mathrm{m}}(\mathrm{cr})$ $\mathrm{kJ\ mol^{-1}}$	$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}(\mathrm{cr})$ $\mathrm{kJ\ mol^{-1}}$	Reference
1	zrm	i-SMB	colorless, CO_2 99.981	8	no	m	−7850.5 ± 1.0	125.2 ± [2.3]	1980SMI/STE
2	na	i-SMB	pale yellow	na	na	na	−7839.8 ± 0.4	114.5 ± [2.1]	1970COX/PIL, 1967WES/WON
3	0.016% ash	i-SMB	light green	11	no	m	−7842.2 ± 3.5	116.9 ± [4.1]	1939RIC/PAR

Recommendation

$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}(\mathrm{cr},\ 298.15\ \mathrm{K})$	$125.2 \pm 2.3\ \mathrm{kJ\ mol^{-1}}$	Suggested value	Entry 1

Evaluation

The enthalpy of formation determined by Smith *et al.* [1980SMI/STE] is the suggested value.

7.16.2. Enthalpy of fusion

TABLE 93. Fusion enthalpy of pyrene

Entry	$\Delta_{\mathrm{trans}}H_{\mathrm{m}}(T_{\mathrm{trans}})$ $\mathrm{kJ\ mol^{-1}}$	T_{trans} K	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ $\mathrm{kJ\ mol^{-1}}$	T_{fus} K	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})^{\mathrm{a}}$ $\mathrm{kJ\ mol^{-1}}$	Method	Purity %	Reference
1	na	na	16.68 ± 1.1	422.4	9.64 ± 2.6	DSC	99.96	2003ROJ/ORO

TABLE 93. Fusion enthalpy of pyrene—Continued

Entry	$\Delta_{trans}H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H^o_m(298\ K)$[a] kJ mol^{-1}	Method	Purity %	Reference
2	na	na	17.11 ± 0.7	424.5	10.0 ± 2.4	DSC	puriss[b]	1973CAS/VEC
3	na	na	15.3 ± 0.2	423	8.2 ± 2.4	DSC	puriss[c]	1972WAU/GET
4	0.29 ± 0.04	120.8	17.36 ± 0.04	423.8	10.2 ± 2.3	AC	99.97	1971WON/WES

[a] Fusion enthalpies adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid pyrene of 311.2 and 227.2 J mol^{-1} K^{-1}, respectively.
[b] Fluka AG, Buchs, Switzerland.
[c] Purissimus, Aldrich Chem. Co.

Recommendation

$\Delta_{fus}H_m\ (T_{fus})$	17.36 ± 0.04 kJ mol^{-1}	Recommended value	Entry 4
$\Delta_{fus}H^o_m(298\ K)$	10.2 ± 2.3 kJ mol^{-1}	Recommended value	Entry 4

Evaluation

Entry 4, the fusion enthalpy measured by adiabatic calorimetry by Wong and Westrum, is recommended [1971WON/WES]. The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an of the uncertainty estimate associated with the temperature adjustment.

7.16.3. Enthalpy of vaporization

TABLE 94. Vaporization enthalpy of pyrene

Entry	T_{Range} K	$\Delta_{vap}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H^o_m(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	298	92.4 ± 1.0	298	92.4 ± 1.0	CGC	98+	2008HAN/NUT
2	na	na	na	87.5 ± 2.6	GC	98+	2006HAF/PAR
3	443	66.1 ± 1.7	443	79.4 ± 2.9	DSC	99.96	2003ROJ/ORO
4	423.8	76.77	423.8	88.2[a]			1998RUZ/MOK
5	413–467	75.6 ± 0.3[b]	441	88.0 ± 2.2[c]	PG	97.0+	1988SAS/JOS
6	513–668	73.0[d]	528	94.0[e]	na	na	1987STE/MAL
7	na	na	na	86.6	GC	na	1984YAM/KUW
8	398–458	76.5 ± 0.52[b,e]	411	86.8 ± 1.8	IPG	Zrm[f]	1980SMI/STE
9	496	86.17 ± 3.2[b]	496	104.2 ± 3.6	P-BP	na	1955TSY

[a] See discussion below.
[b] Calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided in the reference.
[c] Vaporization enthalpies adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity for liquid pyrene of 311.2 J mol^{-1} K^{-1}.
[d] Calculated from the Antoine constants.
[e] Measurements on the supercooled liquid.
[f] Zone refined material.

Recommendation

$\Delta_{vap}H^o_m(298.15\ K)$	89.4 ± 3.1 kJ mol^{-1}	Suggested value	Entries 1,2, 4

Evaluation

A value of 76.77 kJ mol^{-1} at $T=423.8$ K has been recommended by Ruzicka *et al.* in a recent critical evaluation [1998RUZ/MOK]. The recommendation of Ruzicka *et al.* appears to be based on the consistency of vapor pressure measurements and other calorimetric properties measured at the triple point reported in the literature and does not include results of their own vapor pressure measurements. No uncertainty is provided with their recommendation. The suggested value at $T=298.15$ K is the mean of entries 1,2, and 4. These are the most recent measurements and the mean is consistent with the sublimation enthalpy calculated in the last column of Table 97.

7.16.4. Enthalpy of sublimation

TABLE 95. Sublimation enthalpy of pyrene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	322–381	97.8 ± 3.3	352	99.7 ± 3.4	ME	99.0	2008GOL/SUU
2				99.3[a]			1998RUZ/MOK
3	353–393	99.31 ± 0.9[b]	373	102.3 ± 1.5[c]	PG	97+	1988SAS/JOS
4	398–423[d]	93.97 ± 0.4[b]	410	98.4 ± 1.9[c]	IPG	zrm[e]	1980SMI/STE
5	348–419	97.68 ± 0.3	384	100.55 ± 1.9[c]	C	99.0	1974MAL/BAR
6	348–419	97.47 ± 0.7	384	100.34 ± 2.0[e]	ME	99.0	1974MAL/BAR

[a] See comment below.
[b] Calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided in the reference.
[c] Sublimation enthalpy adjusted to 298.15 K using Eq. (3) and an estimated heat capacity of 227.2 J mol^{-1} K^{-1} for solid pyrene.
[d] Measurements on the crystal I state.
[e] Zone refined material.

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	100.3 ± 1.0 kJ mol^{-1}	Recommended value	Entries 1 and 3–6

Evaluation

Pyrene has been recommended as a secondary standard for sublimation enthalpy measurements [1999SAB/XU]. A value of 100.3 ± 3.6 kJ mol^{-1} has been recommended by Pedley *et al.* [1986PED/NAY], the mean value of entries 3–6. A similar value has been recommended by Ruzicka *et al.* [1998RUZ/MOK] in a more recent critical evaluation. The recommendation of Ruzicka *et al.* appears to be based on the consistency of vapor pressure measurements and other calorimetric properties measured at the triple point reported in the literature and does not include results of their own vapor pressure measurements. No uncertainty is provided with their recommendation. In view of the fact that the mean of all six measurements, 100.1 ± 0.9 kJ mol^{-1}, is consitent with both the values recommended by Pedley and Ruzicka *et al.*, the previous recommendation is retained. The mean, excluding entry 2, is 100.3 ± 1.0 kJ mol^{-1}; the uncertainty is reduced, which is consistent with this reproducibility.

TABLE 96. Other sublimation enthalpies reported for pyrene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$[a] kJ mol^{-1}	Method	Purity %	Reference
7	308–398	103.1 ± 6.5	353	105.0 ± 6.5[b]	ME	99.0	1998OJA/SUU
8	313–453	97.9	na	na	GS	99.9	1995NAS/LEN
9	283–323	91.2 ± 0.5	303	91.4 ± 0.5	GS	na	1983SON/ZOL
10	298–363	100.5	330	101.6	ME	na	1958HOY/PEP
11	345–358	94.1	351	95.9	ME	na	1953BRA/CLE
12	351	100.1 ± 1.7	351	101.9 ± 1.8	ME	na	1952INO/SHI

[a] Sublimation enthalpies adjusted to T=298.15 K using Eq. (3) and an estimated heat capacity for solid pyrene of 227.2 J mol^{-1} K^{-1}.
[b] This value was not included in Table 95 because of the magnitude of the uncertainty.

7.16.5. Summary

TABLE 97. A summary of experimental and estimated phase change enthalpies for pyrene

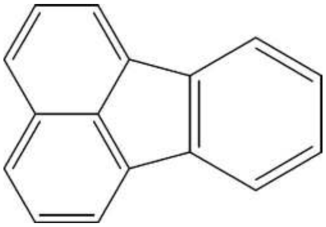
	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.	17.36 ± 0.04	10.2 ± 2.3	89.4 ± 3.1	100.3 ± 1.0	99.6 ± 3.9
estimated	18.1		78.0		96.1[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})$=42.6 J mol^{-1} K^{-1}.

TABLE 98. A summary of suggested enthalpies of sublimation and formation in the condensed and gas phases for pyrene

$\Delta_f H_m^o$(cr, 298.15 K)	$\Delta_{sub} H_m^o$(298.15 K)	$\Delta_f H_m^o$(g, 298.15 K)
kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
125.2 ± 2.3	100.3 ± 1.0	225.5 ± 2.5

7.17. Fluoranthene



Name	Formula	Registry Number	Molecular Weight
Fluoranthene	$C_{16}H_{10}$	[206-44-0]	202.2506 g mol^{-1}

7.17.1. Enthalpy of formation (solid)

TABLE 99. Standard enthalpies of combustion and formation of fluoranthene at T=298.15 K

	Purity						$\Delta_r H_m^o$ (cr)	$\Delta_f H_m^o$ (cr)	
Entry	%	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	kJ mol^{-1}	kJ mol^{-1}	Reference
1	na	SMB	na	na	na	na	−7915.2 ± 0.4	189.9 ± [2.1]	1967WES/WON
2	Purissma Zrm	arc	na	6	no	m	−7917.8 ± 5.4	192.5 ± [5.8]	1965BOY/CHR

Recommendation

$\Delta_f H_m^o$ (cr, 298.15 K)	190.2 ± 2.8 kJ mol^{-1}	Suggested value	Entries 1 and 2

Evaluation

The suggested value is the weighed average of the two available entries.

7.17.2. Enthalpy of fusion

TABLE 100. Fusion enthalpy of fluoranthene

	$\Delta_{fus} H_m(T_{fus})$	T_{fus}	$\Delta_{fus} H_m^o$(298 K)^a		Purity	
Entry	kJ mol^{-1}	K	kJ mol^{-1}	Method	%	Reference
1	18.3^b	na	13.4 ± 1.6	DSC	na	1990HIN/BID
2	18.87 ± 0.6	381.0	14.2 ± 4.7	DSC	purum^c	1973CAS/VEC
3	18.73 ± 0.02	383.3	13.9 ± 1.6	AC	99.94	1971WON/WES

[a] Fusion enthalpy adjusted to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid fluoranthene of 310.5 and 226.6 J mol^{-1} K^{-1}, respectively.

[b] Calculated from the experimental fusion entropy assuming a fusion temperature, T_{fus}=383.3 K.

[c] Fluka AG, Buchs, Switzerland.

Recommendation

$\Delta_{fus} H_m(T_{fus})$	18.73 ± 0.02 kJ mol^{-1}	Recommended value	Entry 3
$\Delta_{fus} H_m^o$ (298.15 K)	13.9 ± 1.6 kJ mol^{-1}	Recommended value	Entry 3

Evaluation

Entry 3, the fusion enthalpy measured by adiabatic calorimetry by Wong and Westrum, is recommended [1971WON/WES]. The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.17.3. Enthalpy of vaporization

TABLE 101. Vaporization enthalpy of fluoranthene

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	86.78 ± 2.6	GC	98+	2006HAF/PAR
2	na	na	na	79.3	CG	99	2002LEI/CHA
3	503–658	61.6[a]	518	87.4 ± 4.5[b]	na	na	1987STE/MAL
4	na	na	na	85.4	GC	na	1984YAM/KUW
5	482–578	76.5 ± 3.2	530	97.6 ± 4.3	P-BP	na	1955TSY

[a] Calculated from the Antoine constants.

[b] Vaporization enthalpies were adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity for liquid fluoranthene of 310.5 J mol^{-1} K^{-1} was calculated from the vapor pressures reported over the temperature range indicated by a Clausius-Clapeyron treatment of the data.

Recommendation

$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}$ (298.15 K)	87.1 ± 3.6 kJ mol^{-1}	Suggested value	Entries 1 and 3

Evaluation

The value chosen is the average of entries 1 and 3; the results of entries 2 and 5 are not consistent with the sublimation enthalpies reported below.

7.17.4. Enthalpy of sublimation

TABLE 102. Sublimation enthalpies of fluoranthene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	327–359	96.9 ± 2.8	343	98.5 ± 2.8	ME	98	2008GOL/SUU
2	313–453	98.3	na	na	GS	99.9	1995NAS/LEN
3	283–328	84.6 ± 1.8	303	84.8 ± 1.8[a]	GS	na	1983SON/ZOL
4	298	99.2 ± 0.8	298	99.2 ± 0.8	C	purum[b]	1972MOR
5	329–354	102.1 ± 2.1	340	103.6 ± 2.2	ME	purissima[c]	1965BOY/CHR
6	298–358	102.6	328	103.6 ± 0.3	ME	mp[d]	1958HOY/PEP

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid fluoranthene of 226.6 J mol^{-1} K^{-1}.

[b] Fluka AG, Buchs, Switzerland.

[c] Aldrich Chemical Co.

[d] Melting point: $T_{\mathrm{fus}=}383.2-383.7$ K.

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}$ (298.15 K)	101.2 ± 2.8 kJ mol^{-1}	Suggested value	Entries 1 and 4–6

Evaluation

The suggested value is the average of entries 1 and 4–6; the uncertainty includes two standard deviations of the mean and an average uncertainty associated with the temperature adjustment. The fusion temperature of fluoranthene is $T_{\mathrm{fus}}=383$ K. The temperature range in 1995NAS/LEN seems inconsistent with a sublimation enthalpy.

7.17.5. Summary

TABLE 103. A summary of experimental and estimated phase change enthalpies for fluoranthene

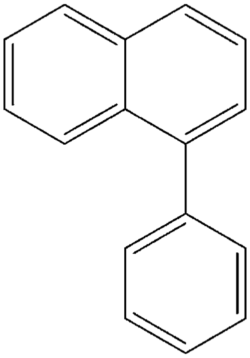
	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)+\Delta_{vap}H_m^o(298\ K)$ kJ mol−1
expt.	18.73 ± 0.02	13.9 ± 1.6	87.1 ± 3.6	101.2 ± 2.8	101.0 ± 3.9
estimated	17.6		78.0		95.6[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=45.8\ J\ mol^{-1}K^{-1}$.

TABLE 104. A summary of suggested enthalpies of sublimation and formation in the condensed and gas phases for fluoranthene

$\Delta_fH_m^o$ (cr, 298.15 K) kJ mol^{-1}	$\Delta_{sub}H_m^o(298.15\ K)$ kJ mol^{-1}	$\Delta_fH_m^o$ (g, 298.15 K) kJ mol^{-1}
190.2 ± 2.8	101.2 ± 2.8	291.4 ± 4.0

7.18. 1-Phenylnaphthalene



Name	Formula	Registry Number	Molecular Weight
1-Phenylnaphthalene	$C_{16}H_{12}$	[605-02-7]	206.282 36 g mol^{-1}

7.18.1. Enthalpy of formation (solid)

None available.

7.18.2. Enthalpy of fusion

None available; $T_{fus}=318$ K.

7.18.3. Enthalpy of vaporization

TABLE 105. Vaporization enthalpy of 1-phenylnaphthalene

Entry	$\Delta_{vap}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	88.6	na	na	GS	99.9	1995NAS/LEN

Evaluation

No experimental details are provided in 1995NAS/LEN. This value is listed as a sublimation enthalpy despite the fact that vapor pressures were measured in the temperature ranges $T=313-453$ K and $T_{fus}=318$ K.

7.18.4. Enthalpy of sublimation

None available.

7.18.5. Summary

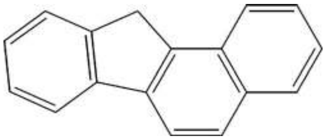
Table 106. A summary of experimental and estimated phase change enthalpies for 1-phenylnaphthalene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K)+ $\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}
expt.			88.6[a]		
estimated	18.7[b]		78.0		

[a]The temperature to which this measurement refers to is not known.

[b]Estimated $\Delta_{tpce}S(T_{fus})$=58.8 J mol^{-1} K^{-1}.

7.19. 11*H*-Benzo[*a*]fluorene



Name	Formula	Registry Number	Molecular Weight
11*H*-benzo[*a*]fluorene, 1,2-benzofluorene	$C_{17}H_{12}$	[238-84-6]	216.277 18 g mol^{-1}

7.19.1. Enthalpy of formation (solid)

None available.

7.19.2. Enthalpy of fusion

Table 107. Fusion enthalpy of 11*H*-benzo[*a*]fluorene

Entry	$\Delta_{trans}H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{tpce}H^o_m$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	3.8 ± 0.6	399.9	18.4 ± 0.2	462.8	12.4 ± 3.3	DSC	na	1979FAR/SHA

[a]Adjustment of the fusion enthalpy to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid 11*H*-benzo[*a*]fluorene of 335.7 and 250.6 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{fus}H_m$ (T_{fus})	18.4 ± 0.2 kJ mol^{-1}	Available value	Entry 1
$\Delta_{tpce}H_m$ (T_{fus})	22.2 ± 0.8 kJ mol^{-1}	Available value	Entry 1
$\Delta_{tpce}H^o_m$ (298.15 K)	12.4 ± 3.3 kJ mol^{-1}	Available value	Entry 1

Evaluation

The total solid to liquid phase change enthalpy was adjusted to T=298.15 K as noted above; the uncertainty in this value includes the standard deviation of the mean (±2σ) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.19.3. Enthalpy of vaporization

Table 108. Vaporization enthalpy of 11*H*-benzo[*a*]fluorene

Entry	T_{Range} K	$\Delta_{vap}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H^o_m$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	83.7	GC	99	2002LEI/CHA

Recommendation

$\Delta_{vap}H^{o}_{m}$ (298.15 K)	83.7 kJ mol^{-1}	Questionable value	Entry 1

Evaluation

Values reported by these authors have been consistently lower than those by other methods.

7.19.4. Enthalpy of sublimation

TABLE 109. Sublimation enthalpy of 11*H*-benzo[*a*]fluorene

Entry	T_{Range} K	$\Delta_{sub}H_{m}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^{o}_{m}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	313–453	105.4	na	na	GS	99.9	1995NAS/LEN

Recommendation

$\Delta_{sub}H^{o}_{m}$ (T)	105.4 kJ mol^{-1}	Questionable value	Entries 1

Evaluation

No experimental details are provided in 1995NAS/LEN.

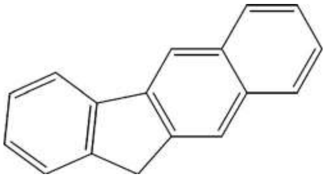
7.19.5. Summary

TABLE 110. A summary of experimental and estimated phase change enthalpies for 11*H*-benzo[*a*]fluorene

	$\Delta_{tpce}H_{m}(T_{fus})$ kJ mol^{-1}	$\Delta_{tpce}H^{o}_{m}$(298 K) kJ mol^{-1}	$\Delta_{vap}H^{o}_{m}$(298 K)^{a} kJ mol^{-1}	$\Delta_{sub}H_{m}$(298 K) kJ mol^{-1}	$\Delta_{tcpe}H^{o}_{m}$(298 K)+ $\Delta_{vap}H^{o}_{m}$(298 K) kJ mol^{-1}
expt.	22.2 ± 0.8	12.4 ± 3.3	83.7	105.4	96.1^{b}
estimated	23.4		82.7		106.1

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=60.6$ J mol^{-1} K^{-1}.
[b] The lack of internal consistency questions the accuracy of the measurements.

7.20. 11*H*-Benzo[*b*]fluorene



Name	Formula	Registry Number	Molecular Weight
11*H*-benzo[*b*]fluorene, 2,3-benzofluorene	$C_{17}H_{12}$	[243-17-4]	216.277 18 g mol^{-1}

7.20.1. Enthalpy of formation (solid)

None available.

7.20.2. Enthalpy of fusion

TABLE 111. Fusion enthalpy of 11*H*-benzo[*b*]fluorene

Entry	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$[a] kJ mol^{-1}	Method	Purity %	Reference
1	23.4 ± 0.6	489.7	12.0 ± 3.8	DSC	na	1979FAR/SHA

[a] Adjustment of the fusion enthalpy to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid 11*H*-benzo[*b*]fluorene of 335.7 and 250.6 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}\ (T_{\mathrm{fus}})$	23.4 ± 0.6 kJ mol^{-1}	Available value	Entry 1
$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	12.0 ± 3.8 kJ mol^{-1}	Available value	Entry 1

Evaluation

The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.20.3. Enthalpy of vaporization

TABLE 112. Vaporization enthalpy of 11*H*-benzo[*b*]fluorene

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H_{m}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	298	97.5 ± 5.8	298	97.5 ± 5.8	CGC	98[a]	2008HAN/NUT
2	na	na	na	84.7	GC	99	2002LEI/CHA

[a] The chromatography generally separates any impurities.

Recommendation

$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	97.5 ± 5.8 kJ mol^{-1}	Available value	Entry 1

Evaluation

This value was chosen because combined with $\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$, a better fit with $\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ is obtained; see Table 114. Values reported by the authors of entry 2 have been consistently lower than those by other methods.

7.20.4. Enthalpy of sublimation

TABLE 113. Sublimation enthalpy of 11*H*-benzo[*b*]fluorene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	344–398	1193 ± 2.6	371	1220 ± 2.8[a]	ME	98.0	1998OJA/SUU
2	313–453	111.2	na	na	GS	99.9	1995NAS/LEN

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid 11*H*-benzo[*b*]fluorene of 250.6 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H_{m}\ (298.15\ \mathrm{K})$	122.0 ± 2.8 kJ mol^{-1}	Available value	Entry 1

Evaluation

No experimental details are provided in 1995NAS/LEN.

7.20.5. Summary

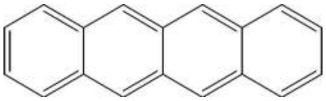
TABLE 114. A summary of experimental and estimated phase change enthalpies for 11*H*-benzo[*b*]fluorene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K)+ $\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}
expt.	23.4 ± 0.6	12.0 ± 3.8	97.5 ± 5.8	122.0 ± 2.8	109.5 ± 6.9^a
estimated	24.8		82.7		107.5^b

[a] The lack of internal consistency questions the accuracy of all measurements.

[b] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus}) = 50.6$ J mol^{-1} K$^{-1.}$

7.21. Naphthacene



Name	Formula	Registry Number	Molecular Weight
Naphthacene, tetracene	$C_{18}H_{12}$	[92-24-0]	228.287 88 g mol^{-1}

7.21.1. Enthalpy of formation (solid)

TABLE 115. Standard enthalpies of combustion and formation of naphthacene at $T = 298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m$(cr) kJ mol^{-1}	$\Delta_f H^o_m$(cr) kJ mol^{-1}	Reference
1	na	i-smb	mp: 350	4	no	m	-9004.9 ± 1.8	$206.7 \pm [3.0]$	2002NAG
2	na	i-SMB	mp: 335–337	4	no	m	-8956.9 ± 1.3	$158.7 \pm [2.7]$	1951MAG/HAR

Recommendation

$\Delta_f H^o_m$ (cr, 298.15 K)	206.7 ± 3.0 kJ mol^{-1}	Questionable value	Entry 1

Evaluation

There is a general consensus among a number of investigators [2004YU/SUM, 1998HER/BIE, 1995POP/HOW, 1987KAO, 1969DEW/DEL] that the experimental enthalpy of formation value by Magnus *et al.* [1951MAG/HAR] for naphthacene is erroneous. Naphthacene rapidly reacts with oxygen to give naphthacenequinone in solution. Thus, it is necessary to handle naphthacene carefully enough to avoid oxidation in sample preparation. It has been suggested [2002NAG] that the sample used for measurements by Magnus *et al.* [1951MAG/HAR] might have been oxidized before the calorimetric measurements. The more recent value by Nagano [2002NAG] is in better agreement with values predicted by quantum chemical calculations. In order to check the self-consistency of the value, the enthalpy of formation in the condensed state of naphthacene was estimated from that for naphthalene, anthracene, phenanthrene and benzo[*a*]anthracene. From the first two, one estimates a solid phase value of 177.0 kJ mol^{-1} and from the last three, 188.2 kJ mol^{-1} [2001SLA/LIE]. Since the experimental values deviate so much from empirical trends, we cannot suggest this value, which should be used with caution.

7.21.2. Enthalpy of fusion

TABLE 116. Fusion enthalpy of naphthacene

Entry	$\Delta_{trans}H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{tpce}H^o_m$(298 K) kJ mol^{-1}	Method	Purity %	Reference
1	1.0	1.4	35.9	623	16.6^a	DSC	na	2002NAG

[a] Adjustment of the total solid-liquid phase change enthalpy to $T = 298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid naphthacene of 353.4 and 261 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\text{tpce}}H_{\text{m}}$ (T_{fus})	36.9 kJ mol^{-1}	Available value	Entry 1
$\Delta_{\text{tpce}}H^{\text{o}}_{\text{m}}$ (298.15 K)	16.6 kJ mol^{-1}	Available value	Entry 1

Evaluation

The total solid-liquid phase change enthalpy was adjusted to T=298.15 K as noted above; the uncertainty in the temperature adjustment amounts to ±6.7 kJ mol^{-1} ($\pm 2\sigma$).

7.21.3. Enthalpy of vaporization

None available.

7.21.4. Enthalpy of sublimation

TABLE 117. Sublimation enthalpy of naphthacene

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	387–472	126.0 ± 9.0	429	131.2 ± 9.2[a]	ME	98	1998OJA/SUU
2	313–453	126.5	na	na	GS	99.9	1995NAS/LEN
3	419–446	128.7 ± 2.0	437	143.7 ± 5.0	TE, ME	97	1980DEK
4	380–476	124.7	428[b]	129.9 ± 3.0[a]	ME	na	1967WAK/INO
5	433–493	129.2	463	135.8 ± 2.2[a]	HSA	na	1965MOR
6	459	132.6 ± 5.0	459	139.1 ± 5.4[a]	HSA	na	1964FIE/MAC
7	459	113.4	459	119.8[a]	ME	mp[c]	1964FIE/MAC, 1952INO/SHI
8	na	124.3	na	na	na	na	1951MAG/BEC

[a] Sublimation enthalpies adjusted to T=298.15 K using Eq. (3) and an estimated heat capacity for solid napthacene of 261 J mol^{-1} K^{-1}.
[b] Temperature range approximate.
[c] Characterized by melting point: 613 K.

Recommendation

$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$ (298.15 K)	135.9 ± 5.1 kJ mol^{-1}	Available value	Entries 1 and 3–6

Evaluation

The value is the mean of entries 1 and 3–6; the uncertainty represents two standard deviations of the mean and an uncertainty of 1.5 kJ mol^{-1} associated with the temperature adjustment. No experimental details are provided in 1995NAS/LEN. If no uncertainty is associated with $\Delta_{\text{sub}}H_{\text{m}}(T/\text{K})$, then the uncertainty associated with $\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$(298.15 K) is due solely to the temperature adjustment.

7.21.5. Summary

TABLE 118. A summary of experimental and estimated phase change enthalpies for naphthacene

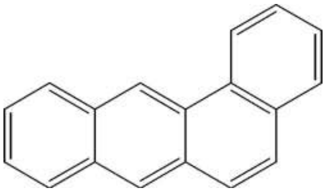
	$\Delta_{\text{tpce}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{tpce}}H^{\text{o}}_{\text{m}}$(298 K) kJ mol^{-1}	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}$(298 K) kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$(298 K) kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}$(298 K)+ $\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}$(298 K) kJ mol^{-1}
expt.	36.9	16.6		135.9 ± 5.1	
estimated	25.5		87.4		112.9[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\text{tpce}}S(T_{\text{fus}})$=43.8 J mol^{-1} K^{-1}.

TABLE 119. A summary of available experimental enthalpies of sublimation and formation in the condensed and gas phases for naphthacene

$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}$ (cr, 298.15 K) kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$(298.15 K) kJ mol^{-1}	$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}$ (g,298.15 K) kJ mol^{-1}
206.7 ± 3.0	135.9 ± 5.1	342.6 ± 5.9

7.22. Benz[*a*]anthracene



Name	Formula	Registry Number	Molecular Weight
Benz[*a*]anthracene, 1,2-benzanthracene	$C_{18}H_{12}$	[56-55-3]	228.287 88 g mol^{-1}

7.22.1. Enthalpy of formation (solid)

TABLE 120. Standard enthalpies of combustion and formation of benz[*a*]anthracene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H_m^o$(cd) kJ mol^{-1}	$\Delta_f H_m^o$(cd) kJ mol^{-1}	Reference
1	na	SMB	na	4	na	m	-8969.0 ± 2.3	$170.8 \pm [3.3]$	1970COX/PIL, 1951MAG/HAR

Recommendation

$\Delta_f H_m^o$ (cr, 298.15 K)	170.8 ± 3.3 kJ mol^{-1}	Available value	Entry 1

Evaluation

The available experimental value, given by Magnus *et al.* [1951MAG/HAR], was analyzed and recalculated by Cox and Pilcher [1970COX/PIL].

7.22.2. Enthalpy of fusion

TABLE 121. Fusion enthalpy of benz[*a*]anthracene

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H_m^o(298\ K)^a$ kJ mol^{-1}	Method	Purity %	Reference
1	22.3	431.2	14.0	DSC	99	1995HAI/SAN
2	21.4 ± 0.3	434.3	12.9 ± 2.8	DSC	SMG[b]	1973CAS/VEC

[a] Fusion enthalpy adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid of benz[*a*]anthracene of 353.4 and 261 J mol^{-1} K^{-1}, respectively.

[b] From Schuchard, München, Germany.

Recommendation

$\Delta_{fus}H_m$ (T_{fus})	21.4 ± 0.3 kJ mol^{-1}	Suggested value	Entry 2
$\Delta_{fus}H_m^o$ (298.15 K)	12.9 ± 2.8 kJ mol^{-1}	Suggested value	Entry 2

Evaluation

The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean $(\pm 2\sigma)$ as well as an estimate of the uncertainty associated with the temperature adjustment.

7.22.3. Enthalpy of vaporization

TABLE 122. Vaporization enthalpy of benz[*a*]anthracene

Entry	T_{Range} K	$\Delta_{\text{vap}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	298	105.8 ± 3.8	298	105.8 ± 3.8	CGC	99	2008HAN/NUT
2	na	na	na	96.9 ± 2.8	GC	99	2006HAF/PAR

Recommendation

$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$	105.8 ± 3.8 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

This value was chosen because combined with $\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$, a better fit with $\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$, is obtained; see Table 124.

7.22.4. Enthalpy of sublimation

TABLE 123. Sublimation enthalpy of benz[*a*]anthracene

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	313–453	115.5	na	na	GS	99.9	1995NAS/LEN
2	377–426	108.0	389	111.6[a]	na	na	1987STE/MAL
3	283–323	81.3 ± 5.0	303	81.5 ± 5.0[a]	GS	na	1983SON/ZOL
4	377–425	104 ± 4.0	402	108.1 ± 4.2[a]	TE	99.9	1983FER/IMP
5	373–396	113.5 ± 2.0	386	123.3 ± 6.0	TE, ME	98+	1980DEK
6	330–390	113.4 ± 1.4	360	115.9 ± 1.5[a]	ME	98.4	1974MUR/POT
7	365–450	120.5	405[b]	124.8[a]	ME	na	1967WAK/INO
8	377–400	104.5	389	108.2[a]	ME	na	1964KEL/RIC
9	317–383	119.7	350	121.7[a]	ME	na	1958HOY/PEP
10	na	109.2	na	na	na	na	1951MAG/BEC

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid benz[*a*]anthracene of 261 J mol^{-1} K^{-1}

[b] Temperature range approximate

Recommendation

$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$	119.5 ± 5.0 kJ mol^{-1}	Suggested value	Entries 2, 5–7, 9

Evaluation

This value is the mean of entries 2, 5–7, and 9. The uncertainty represents two standard deviations of the mean. Despite the large uncertainty, this value seems consistent with the sublimation enthalpy obtained indirectly.

7.22.5. Summary

TABLE 124. A summary of experimental and estimated phase change enthalpies for benz[*a*]anthracene

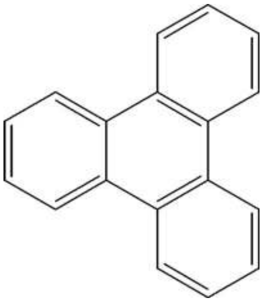
	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\text{ K})+\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}
expt.	21.4 ± 0.3	12.9 ± 2.8	105.8 ± 3.8	119.5 ± 5.0	118.7 ± 4.7
estimated	19.0		87.4		106.4[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\text{tpce}}S(T_{\text{fus}})=43.8$ J mol^{-1} K^{-1}.

TABLE 125. A summary of available experimental enthalpies of sublimation and formation in the condensed and gas phases for benzo[*a*]anthracene

$\Delta_f H_m^o$ (cr, 298.15 K)	$\Delta_{sub} H_m^o$(298.15 K)	$\Delta_f H_m^o$ (g, 298.15 K)
kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
170.8 ± 3.3	119.5 ± 5.0	290.3 ± 6.0

7.23. Triphenylene



Name	Formula	Registry Number	Molecular Weight
Triphenylene, 9,10-benzophenanthrene	$C_{18}H_{12}$	[217-59-4]	228.287 88 g mol^{-1}

7.23.1. Enthalpy of formation (solid)

TABLE 126. Standard enthalpies of combustion and formation of triphenylene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_c H_m^o$(cr) kJ mol^{-1}	$\Delta_f H_m^o$(cr) kJ mol^{-1}	Reference
1	na	RMB	CO_2 recovery 99.998%	8	no	m	−8949.9 ± 1.2	151.8 ± [2.6]	1978GOO
2	na	SMB	na	na	na	na	−8939.2 ± 0.5	141.0 ± [2.4]	1967WES/WON
3	na	SMB	mp: 468−469 K	4	no	m	−8945.4 ± 2.2	147.2 ± [3.2]	1951MAG/HAR

Recommendation

$\Delta_f H_m^o$ (cr, 298.15 K)	150.0 ± 2.9 kJ mol^{-1}	Suggested value	Entries 1 and 3

Evaluation

The suggested value is the weighted average of the available data of Good [1978GOO] and Magnus *et al.* [1951MAG/HAR].

7.23.2. Enthalpy of fusion

TABLE 127. Fusion enthalpy of triphenylene

Entry	$\Delta_{fus} H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus} H_m^o$(298 K)^a kJ mol^{-1}	Method	Purity %	Reference
1	25.1 ± 0.9	473.8	14.1 ± 3.7	DSC	SMG^b	1973CAS/VEC
2	24.74 ± 0.01	471.0	13.9 ± 3.6	AC	99.96	1971WON/WES

[a] Fusion enthalpy adjusted to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid triphenylene of 353.4 and 261 J mol^{-1} K^{-1}, respectively

[b] From Schuchard, München, Germany.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$	24.74 ± 0.01 kJ mol^{-1}	Recommended value	Entry 2
$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	13.9 ± 3.6 kJ mol^{-1}	Recommended value	Entry 2

Evaluation

The fusion enthalpy measured by adiabatic calorimetry by Wong and Westrum [1971WON/WES] is recommended. The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes an estimate of the uncertainty associated with the temperature adjustment.

7.23.3. Enthalpy of vaporization

TABLE 128. Vaporization enthalpy of triphenylene

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	298	106.1 ± 7.8	298	106.1 ± 7.8	CGC	98[a]	2008HAN/NUT
2	na	na	na	88.5	GC	99	2002LEI/CHA
3	600–720	67.5	660	104.6 ± 6[b]	na	na	1987STE/MAL
4	na	na	na	99.6	GC	na	1984YAM/KUW

[a] The chromatography generally separates any impurities.
[b] Vaporization enthalpies adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity for liquid triphenylene of 353.4 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	106.1 ± 7.8 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The vaporization enthalpy of the third entry was adjusted using Eq. (2) over a large temperature range; the results should be treated cautiously. Values reported by the authors of entry 2 have been consistently lower than those by other methods.

7.23.4. Enthalpy of sublimation

TABLE 129. Sublimation enthalpy of triphenylene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	368–399	124.8 ± 5.8	384	128.2 ± 5.9	ME	97+	2008GOL/SUU
2	313–453	114.5	na	na	GS	99.9	1995NAS/LEN
3	381–406	115.6 ± 2.0	395	119.5 ± 2.4	TE, ME	98	1980DEK
4	370–500	107.1	430[b]	112.4	ME	na	1967WAK/INO
5	338–398	117.8 ± 4	368	120.6 ± 4.1	ME	na	1958HOY/PEP
6	na	110.0	na	na	na	na	1951MAG/BEC

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid triphenylene of 261 J mol^{-1} K^{-1}.
[b] Temperature range approximate.

Recommendation

$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$ (298.15 K)	120.1 ± 3.3 kJ mol^{-1}	Suggested value	Entries 2 and 4

Evaluation

The mean of entries 3 and 5 is suggested; the uncertainty of the suggested value represents the mean of the uncertainties of both values.

7.23.5. Summary

TABLE 130. A summary of suggested experimental and estimated phase change enthalpies for triphenylene

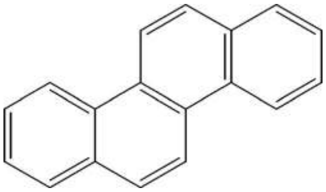
	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K)+ $\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}
expt.	24.74 ± 0.01	13.9 ± 3.6	106.1 ± 7.8	120.1 ± 3.3	120.0 ± 8.6
estimated	20.6		87.4		108.0[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=43.8$ J mol^{-1} K^{-1}.

TABLE 131. A summary of suggested enthalpies of sublimation and formation in the condensed and gas phases of triphenylene

$\Delta_f H^o_m$ (cr,298.15 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298.15 K) kJ mol^{-1}	$\Delta_f H^o_m$ (g, 298.15 K) kJ mol^{-1}
150.0 ± 2.9	120.1 ± 3.3	270.1 ± 4.4

7.24. Chrysene



Name	Formula	Registry Number	Molecular Weight
Chrysene, benzo[*a*]phenanthrene	$C_{18}H_{12}$	[218-01-9]	228.28 788 g mol^{-1}

7.24.1. Enthalpy of formation (solid)

TABLE 132. Standard enthalpies of combustion and formation of chrysene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m$ (cr) kJ mol^{-1}	$\Delta_f H^o_m$ (cr) kJ mol^{-1}	Reference
1	na	i-SMB	mp: 255–256	6	no	m	−8943.5 ± 2.1	145.3 ± 2.2	1951MAG/HAR

Recommendation

$\Delta_f H^o_m$ (cr, 298.15 K)	145.3 ± 2.2 kJ mol^{-1}	Available value	Entry 1

Evaluation

The available value given by Magnus *et al.* [1951MAG/HAR] was analyzed and recalculated by Cox and Pilcher [1970COX/PIL]. In order to check the self-consistency of the value, the enthalpy of formation in the condensed state of chrysene was estimated from that for naphthalene and phenanthrene. An estimate of 142.2 kJ mol^{-1} was obtained, in good agreement with the experimental value determined by Magnus.

7.24.2. Enthalpy of fusion

TABLE 133. Total phase change enthalpy of chrysene

Entry	$\Delta_{trans}H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{tpce}H^o_m$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	3.22 ± 0.4	512	26.15 ± 0.17	531.4	14.8 ± 4.8	DSC	purum[b]	1973CAS/VEC

[a] Total phase change enthalpy adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid chrysene of 353.4 and 261 J mol^{-1} K^{-1}, respectively.

[b] Fluka AG, Buchs, Switzerland.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}$ (T_{fus})	26.2 ± 0.2 kJ mol^{-1}	Suggested value	Entry 1
$\Delta_{\mathrm{tpce}}H^{\mathrm{o}}_{\mathrm{m}}$ (298.15 K)	14.8 ± 4.8 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.24.3. Enthalpy of vaporization

TABLE 134. Vaporization enthalpy of chrysene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	298	106.2 ± 8.6	298	106.2 ± 8.6	CGC	98$^{\mathrm{a}}$	2008ZHA/UNH
2	na	na	na	96.7 ± 2.8	GC	98+	2006HAF/PAR
3	na	na	na	89.6	GC	99	2002LEI/CHA

[a] The chromatography generally separates any impurities.

Recommendation

$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$ (298.15 K)	106.2 ± 8.6 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The first entry was chosen on the basis of how well the $\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K) and $\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K) reproduced $\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K). Values reported by the authors of entry 3 have been consistently lower than those by other methods.

7.24.4. Enthalpy of sublimation

TABLE 135. Sublimation enthalpy of chrysene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K)$^{\mathrm{a}}$ kJ mol^{-1}	Method	Purity %	Reference
1	372–409	109.9 ± 7.2	391	114.4 ± 7.3	ME	97+	2008GOL/SUU
2	313–453	118.8	na	na	GS	99.9	1995NAS/LEN
3	na	na	na	99.6	GC	na	1984YAM/KUW
4	390–417	118.9 ± 4	406	123.2 ± 4.2	TE, ME	na$^{\mathrm{b}}$	1980DEK
5	360–460	117.6	410$^{\mathrm{c}}$	122.1	ME	na	1967WAK/INO
6	353–418	121.4	385	124.8	ME	mp$^{\mathrm{d}}$	1958HOY/PEP
7	na	117.5	na	na	na	na	1951MAG/BEC

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid chrysene of 261 J mol^{-1} K^{-1}.

[b] Source: Merck.

[c] Temperature range approximate.

[d] Characterized by melting point: 528.2–529.2 K

Recommendation

$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$ (298.15 K)	123.4 ± 4.2 kJ mol^{-1}	Suggested value	Entries 4 6

Evaluation

There is no supporting experimental information in 1995NAS/LEN; it is not clear whether the results reported in this work refer to $T=298.15$ K. The value suggested is the average of entries 2–4; the uncertainty is derived from the uncertainty of the second entry.

7.24.5. Summary

TABLE 136. A summary of experimental and estimated phase change enthalpies of chrysene

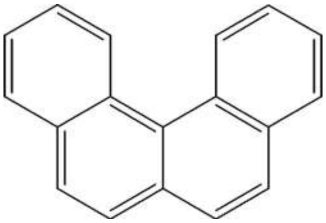
	$\Delta_{\mathrm{tpce}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.	29.4	14.8 ± 4.8	106.2 ± 8.6	123.4 ± 4.2	121.0 ± 9.8
estimated	23.3		87.4		110.7[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=43.8\ \mathrm{J\ mol^{-1}\ K^{-1}}$.

TABLE 137. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of chrysene

$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}$ (cr, 298.15 K) kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}$ (g, 298.15 K) kJ mol^{-1}
145.3 ± 2.2	123.4 ± 4.2	268.7 ± 4.7

7.25. Benzo[*c*]phenanthrene



Name	Formula	Registry Number	Molecular Weight
Benzo[*c*]phenanthrene, 3,4-benzophenanthrene	$C_{18}H_{12}$	[195-19-7]	228.287 88 g mol^{-1}

7.25.1. Enthalpy of formation (solid)

TABLE 138. Standard enthalpies of combustion and formation of benzo[*c*]phenanthrene at *T*=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_{\mathrm{r}}H^{\mathrm{o}}_{\mathrm{m}}$ (cr) kJ mol^{-1}	$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}$ (cr) kJ mol^{-1}	Reference
1	na	SMB	na	5	na	m	−8983.0 ± 1.9	184.9 ± [3.0]	1970COX/PIL, 1951MAG/HAR

Recommendation

$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}$ (cr, 298.15 K)	184.9 ± 3.0 kJ mol^{-1}	Available value	Entry 1

Evaluation

The experimental value given by Magnus *et al.* [1951MAG/HAR] was analyzed and recalculated by Cox and Pilcher [1970COX/PIL].

7.25.2. Enthalpy of fusion

TABLE 139. Fusion enthalpy of benzo[*c*]phenanthrene

Entry	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\text{fus}}H^{\circ}_{\text{m}}(298\text{ K})^{a}$ kJ mol^{-1}	Method	Purity %	Reference
1	16.3 ± 1.4	334.8	14.0 ± 1.6	DSC	na	1973CAS/VEC

[a] Adjustment of the fusion enthalpy to $T=298.15$ K using Eq.(5) and estimated heat capacities for liquid and solid benzo[*c*]phenanthrene of 353.4 and 261 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$	16.3 ± 1.4 kJ mol^{-1}	Available value	Entry 1
$\Delta_{\text{fus}}H^{\circ}_{\text{m}}(298.15\text{ K})$	14.0 ± 1.6 kJ mol^{-1}	Available value	Entry 1

Evaluation

The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the measurements $(\pm 2\sigma)$ as well as an estimate of the uncertainty associated with the temperature adjustment.

7.25.3. Enthalpy of vaporization

None available.

7.25.4. Enthalpy of sublimation

TABLE 140. Sublimation enthalpy of benzo[*c*]phenanthrene

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\circ}_{\text{m}}(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	na	106.3	na	na	na	na	1967WAK/INO, 1951MAG/BEC

Recommendation

$\Delta_{\text{sub}}H^{\circ}_{\text{m}}(\bar{T})$	106.3 kJ mol^{-1}	Questionable value	Entry 1

7.25.5. Summary

TABLE 141. A summary of experimental and estimated phase change enthalpies of benzo[*c*]phenanthrene

	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\circ}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{vap}}H^{\circ}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{sub}}H^{\circ}_{\text{m}}(\bar{T}\text{ K})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\circ}_{\text{m}}(298\text{ K})+\Delta_{\text{vap}}H^{\circ}_{\text{m}}(298\text{ K})$ kJ mol^{-1}
expt.	16.3 ± 1.4	14.0 ± 1.6		106.3	
estimated	14.7		87.4		102.1[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\text{tpce}}S(T_{\text{fus}})=43.8$ J mol^{-1} K^{-1}.

TABLE 142. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of benzo[*c*]phenanthrene

$\Delta_{\text{f}}H^{\circ}_{\text{m}}$ (cr, 298.15 K) kJ mol^{-1}	$\Delta_{\text{sub}}H^{\circ}_{\text{m}}(\bar{T}\text{ K})$ kJ mol^{-1}	$\Delta_{\text{f}}H^{\circ}_{\text{m}}(\text{g},\bar{T}\text{ K})$ kJ mol^{-1}
184.9 ± 3.0	106.3	291.2

7.26. *p*-Terphenyl

Name	Formula	Registry Number	Molecular Weight
p-Terphenyl	$C_{18}H_{14}$	[92-94-4]	230.303 76 g mol^{-1}

7.26.1. Enthalpy of formation (solid)

TABLE 143. Standard enthalpies of combustion and formation of *p*-terphenyl at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H_m^o$(cd) kJ mol^{-1}	$\Delta_f H_m^o$(cd) kJ mol^{-1}	Reference
1	>99.9	smb	GC	9	no	m	−9242.8 ± 2.4	158.8 ± 3.4	2008RIB/SAN
2	>99.99	SMB	DSC, glc	5	oil	m	−9236.4 ± 0.9	152.5 ± [2.5]	1997VER
3	na	SMB	na	na	na	na	−9246.6 ± 4.6	162.6 ± [5.2]	2005AFE/LIE, 1977BAL/LEB

Recommendation

$\Delta_f H_m^o$ (cr, 298.15 K)	158.8 ± 3.4 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The suggested value is the one reported by Ribeiro da Silva *et al.* [2008RIB/SAN]. The selection of this value is supported by the fact that the value determined by Verevkin [1997VER] seemed to be 9 kJ mol^{-1} too low when a plot of the enthalpies of formation in the condensed state of benzene, biphenyl, and *p*-terphenyl as a function of the number of phenyl rings is carried out [2001SLA/LIE].

7.26.2. Enthalpy of fusion

TABLE 144. Fusion enthalpy of *p*-terphenyl

Entry	$\Delta_{trans}H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H_m^o$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	na	na	35.3 ± 0.4	482.4	23.6 ± 3.9	DSC	99.99	1997VER
2	0.304	193	na	na	na	AC	99.9+	1988SAI/ATA
3	na	na	35.3	487	23.4	AC	99.9+	1983CHA
4	na	na	41.6 ± 1.6	493.1	29.3	DSC	zr[b]	1982WAS/RAD
5	na	na	35.5 ± 2.6	486.3	23.6 ± 4.7	DSC	na	1979SMI
6	0.095	193	na	na	na	AC	zr[b]	1979CAI/DWO

[a] Fusion enthalpies adjusted to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid *p*-terphenyl of 366.4 and 279 J mol^{-1} K^{-1}, respectively.
[b] Zone refined.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	35.4 ± 0.1 kJ mol^{-1}	Recommended value	Entries 1, 3, 5
$\Delta_{fus}H_m^o$ (298.15 K)	23.5 ± 3.9 kJ mol^{-1}	Recommended value	Entries 1, 3, 5

Evaluation

The value recommended for $\Delta_{fus}H_m(T_{fus})$ is an average of entries 1, 3, and 5. The uncertainty is two standard deviations of the mean. The fusion enthalpy was adjusted to 298.15 K as noted above; a mean temperature of 485 K was used. The uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.26.3. Enthalpy of vaporization

TABLE 145. Vaporization enthalpy of *p*-terphenyl

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	298	99.5 ± 8.8^{a}	298	99.5 ± 8.8^{a}	CGC	99	2008HAN/NUT
2	na	na	na	79.2	GC	99	2002LEI/CHA
3	499–700	70.9^{b}	600	102.8 ± 5.0^{c}	na	na	1987STE/MAL

[a] Measurements made on *p*-terphenyl-d$_{14}$.
[b] Calculated from the Antoine constants.
[c] Vaporization enthalpy adjusted to T=298.15 K using Eq.(2) and an estimated heat capacity of 366.4 J mol^{-1} K^{-1} for liquid *p*-terphenyl.

Recommendation

$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	101.2 ± 6.9 kJ mol^{-1}	Suggested value	Entries 1 and 3

Evaluation

The average of entries 1 and 3 is chosen on the basis of how well the sublimation enthalpy is reproduced. The uncertainty associated with the temperature adjustment to T=298.15 K of entry 3 was estimated as ±5.0 kJ mol^{-1}; note that the temperature adjustment is significant. Values reported by the authors of entry 2 have been consistently lower than those by other methods.

7.26.4. Enthalpy of sublimation

TABLE 146. Sublimation enthalpy of *p*-terphenyl

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	373–395	122.6 ± 0.6	384	125.6 ± 1.6	ME	99	2008RIB/SAN
2	353–383	116.2 ± 4.8	368	120.4 ± 4.9	GS	99.99	1997VER
3	338–431	118.9	385	122.6^{a}	na	na	1987STE/MAL
4	338–431	118.4	385^{b}	122.6	ME	na^{c}	1967WAK/INO
5	333–393	120.6	363	123.4	ME	na	1958HOY/PEP

[a] Sublimation enthalpy adjusted to T=298.15 K using Eq. (3) an estimated heat capacity for solid *p*-terphenyl of 279 J mol^{-1} K^{-1}.
[b] Temperature range approximate.
[c] An independent analysis of composition other than a physical property such as melting point is not available.

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	125.6 ± 1.6 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The value suggested is the value reported in 2008RIB/SAN. Entry 3 is probably from 1967WAK/INO.

7.26.5. Summary

TABLE 147. A summary of experimental and estimated phase change enthalpies of *p*-terphenyl

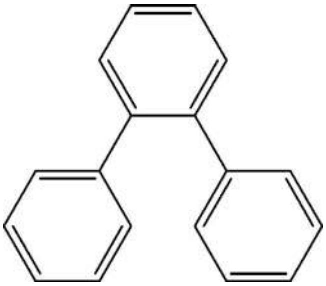
	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.	35.4 ± 0.1	23.5 ± 3.9	101.2 ± 6.9	125.6 ± 1.6	124.7 ± 7.9
estimated	35.8		87.4		123.2^{a}

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=73.6$ J mol^{-1} K^{-1}.

TABLE 148. A summary of suggested enthalpies of sublimation and formation in the condensed and gas phases of *p*-terphenyl

$\Delta_f H^o_m$(cd, 298.15 K)	$\Delta_{sub} H^o_m$(298.15 K)	$\Delta_f H^o_m$(g, 298.15 K)
kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
158.8 ± 3.4	125.6 ± 1.6	284.4 ± 3.8

7.27. *o*-Terphenyl



Name	Formula	Registry Number	Molecular Weight
o-Terphenyl	$C_{18}H_{14}$	[84-15-1]	230.303 76 g mol^{-1}

7.27.1. Enthalpy of formation (solid)

TABLE 149. Standard enthalpies of combustion and formation of *o*-terphenyl at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_c H^o_m$(cr) kJ mol^{-1}	$\Delta_f H^o_m$(cr) kJ mol^{-1}	Reference
1	>99.9	smb	GC	10	Benzoic acid	m	−9266.5 ± 2.8	182.5 ± 3.6	2008RIB/SAN
2	>99.99	SMB	DSC, glc	4	oil	m	−9262.3 ± 1.2	178.3 ± 2.7	1997VER

Recommendation

$\Delta_f H^o_m$ (cr, 298.15 K)	179.8 ± 3.1 kJ mol^{-1}	Suggested value	Entries 1 and 2

Evaluation

The two values agree within the combined uncertainty intervals. The suggested value is the weighed average of the two available values.

7.27.2. Enthalpy of fusion

TABLE 150. Fusion enthalpy of *o*-terphenyl

Entry	$\Delta_{fus} H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus} H^o_m$(298 K)^a kJ mol^{-1}	Method	Purity %	Reference
1	16.9 ± 0.4	327.8	15.0 ± 0.7	DSC	99.99	1997VER
2	17.19 ± 0.01	329.4	15.2 ± 0.65	AC	99.999	1972CHA/BES

[a] Fusion enthalpy adjusted to T=298.15 K using Eq.(5) and estimated heat capacities for liquid and solid *o*-terphenyl of 366.4 and 279 kJ mol^{-1} K^{-1}, respectively.

Recommendation

$\Delta_{fus} H_m$ (T_{fus})	17.19 ± 0.01 kJ mol^{-1}	Recommended value	Entry 2
$\Delta_{fus} H^o_m$ (298.15 K)	15.2 ± 0.7 kJ mol^{-1}	Recommended value	Entry 2

Evaluation

The value from entry 2 measured by adiabatic calorimetry is recommended. The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean $(\pm 2\sigma)$ as well as an estimate of the uncertainty associated with the temperature adjustment.

7.27.3. Enthalpy of vaporization

TABLE 151. Vaporization enthalpy of *o*-terphenyl

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	336–368	81.0 ± 0.9	352	84.2 ± 0.9	GS	99.99	1997VER
2	343–462	77.6 ± 1.6	402	88.6 ± 1.6	EM	99	1989SAS/NGU
3	462–650	63.2	556	90.5[a]	na	na	1987STE/MAL

[a] Vaporization enthalpy adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity of 366.4 J mol^{-1} K^{-1} for liquid *o*-terphenyl.

[b] Calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided in the reference.

Recommendation

$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}$ (298.15 K)	86.4 ± 4.4 kJ mol^{-1}	Suggested value	Entries 1 and 2

Evaluation

The suggested value is the mean of the first two entries; the uncertainty represents two standard deviations of the mean. The third entry has a large temperature adjustment.

7.27.4. Enthalpy of sublimation

TABLE 152. Sublimation enthalpy of *o*-terphenyl

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	312–329	102.3 ± 0.8	321	103.0 ± 0.8	ME	99	2008RIB/SAN

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}$ (298.15 K)	103.0 ± 0.8 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The value is consistent with the sublimation enthalpy calculated from experimental vaporization and fusion enthalpies; see below.

7.27.5. Summary

TABLE 153. A summary of experimental and estimated phase change enthalpies of *o*-terphenyl

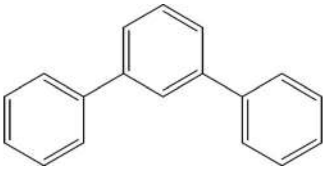
	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt	17.19 ± 0.01	15.2 ± 0.7	86.4 ± 4.4	103.0 ± 0.8	101.6 ± 4.5
estimated	24.2		87.4		111.6[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=73.6$ J mol^{-1} K^{-1}.

TABLE 154. A summary of suggested enthalpies of sublimation and formation in the condensed and gas phase of *o*-terphenyl

$\Delta_f H^o_m(\mathrm{cr}, 298.15\ \mathrm{K})$	$\Delta_{\mathrm{sub}} H^o_m(298.15\ \mathrm{K})$	$\Delta_f H^o_m(\mathrm{g}, 298.15\ \mathrm{K})$
kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
179.8 ± 3.1	103.0 ± 0.8	282.8 ± 3.2

7.28. *m*-Terphenyl



Name	Formula	Registry Number	Molecular Weight
m-Terphenyl	$C_{18}H_{14}$	[92-06-8]	230.30376 g mol^{-1}

7.28.1. Enthalpy of formation (solid)

TABLE 155. Standard enthalpies of combustion and formation of *m*-terphenyl at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m(\mathrm{cr})$ kJ mol^{-1}	$\Delta_f H^o_m(\mathrm{cr})$ kJ mol^{-1}	Reference
1	>99.9	smb	GC	13	Benzoic acid	m	-9245.3 ± 3.0	161.3 ± 3.8	2008RIB/SAN
2	>99.99	SMB	DSC, glc	5	oil	m	-9245.7 ± 1.2	161.7 ± 2.7	1997VER

Recommendation

$\Delta_f H^o_m$ (cr, 298.15 K)	(161.6 ± 3.1) kJ mol^{-1}	Recommended value	Entries 1 and 2

Evaluation

The values are in excellent agreement. The recommended value is the weighed average of the two values.

7.28.2. Enthalpy of fusion

TABLE 156. Fusion enthalpy of *m*-terphenyl

Entry	$\Delta_{\mathrm{fus}} H_m(T_{\mathrm{fus}})$ kJ mol^{-1}	T_{fus}/K	$\Delta_{\mathrm{fus}} H^o_m(298\ \mathrm{K})$[a] kJ mol^{-1}	Method	Purity %	Reference
1	31.0 ± 0.4	361.2	27.0 ± 1.4	DSC	99.99	1997VER
2	22.6	360	18.7	na	na	1971KAM/MIT

[a] Fusion enthalpy adjusted to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid *m*-terphenyl of 366.4 and 279 J mol^{-1} K^{-1}, respectively.

Recommendation

$\Delta_{\mathrm{fus}} H_m$ (T_{fus})	31.0 ± 0.4 kJ mol^{-1}	Suggested value	Entry 1
$\Delta_{\mathrm{fus}} H^o_m$ (298.15 K)	27.0 ± 1.4 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

Entry 1 is the suggested value; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.28.3. Enthalpy of vaporization

TABLE 157. Vaporization enthalpy of *m*-terphenyl

Entry	T_{Range} K	$\Delta_{\text{vap}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{vap}}H_{\text{m}}^{\text{o}}(298.15\text{ K})^{\text{a}}$ kJ mol^{-1}	Method	Purity %	Reference
1	462–691	76.1$^{\text{a}}$	577	98.8$^{\text{b}}$	na	na	1987STE/MAL

[a] Calculated from the Antoine constants.

[b] Vaporization enthalpy adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity of 366.4 J mol^{-1} K^{-1} for liquid *m*-terphenyl.

Recommendation

$\Delta_{\text{vap}}H_{\text{m}}^{\text{o}}$ (298.15 K)	98.8 kJ mol^{-1}	Questionable value	Entry 1

Evaluation

Note the large temperature adjustment.

7.28.4. Enthalpy of sublimation

TABLE 158. Sublimation enthalpy of *m*-terphenyl

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H_{\text{m}}^{\text{o}}(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	337–359	117.0 ± 1.0	348	118.6 ± 1.4	ME	99	2008RIB/SAN
2	329–353	115.5 ± 3.2	341	118.1 ± 3.3	GS	99.99	1997VER
3	313–363	118.9	338	120.6	ME	na	1958HOY/PEP

Recommendation

$\Delta_{\text{sub}}H_{\text{m}}^{\text{o}}$(298.15 K)	118.4 ± 2.4 kJ mol^{-1}	Recommended value	Entries 1 and 2

Evaluation

The recommended value is the mean of both results. The uncertainty is the average uncertainty.

7.28.5. Summary

TABLE 159. A summary of experimental and estimated phase change enthalpies of *m*-terphenyl

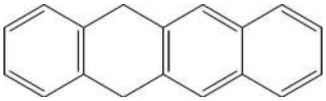
	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{fus}}H_{\text{m}}^{\text{o}}$(298 K) kJ mol^{-1}	$\Delta_{\text{vap}}H_{\text{m}}^{\text{o}}$(298 K) kJ mol^{-1}	$\Delta_{\text{sub}}H_{\text{m}}^{\text{o}}$(298 K) kJ mol^{-1}	$\Delta_{\text{fus}}H_{\text{m}}^{\text{o}}$(298 K) + $\Delta_{\text{vap}}H_{\text{m}}^{\text{o}}$(298 K) kJ mol^{-1}
expt.	31.0 ± 0.4	27.0 ± 1.4	98.8	118.4 ± 2.4	125.8
estimated	26.6		87.4		114.0$^{\text{a}}$

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\text{tpce}}S(T_{\text{fus}})=37.6$ J mol^{-1} K^{-1}.

TABLE 160. A summary of recommended enthalpies of sublimation and formation in the condensed and gas phases of *m*-terphenyl

$\Delta_{\text{f}}H_{\text{m}}^{\text{o}}$(cr, 298.15 K) kJ mol^{-1}	$\Delta_{\text{sub}}H_{\text{m}}^{\text{o}}$(298.15 K) kJ mol^{-1}	$\Delta_{\text{f}}H_{\text{m}}^{\text{o}}$(g, 298.15 K) kJ mol^{-1}
161.6 ± 3.1	118.4 ± 2.4	280.0 ± 3.9

7.29. 5,12-Dihydrotetracene



Name	Formula	Registry Number	Molecular Weight
5,12-Dihydrotetracene	$C_{18}H_{14}$	[959-02-4]	230.3076 g mol^{-1}

7.29.1. Enthalpy of formation (solid)

TABLE 161. Standard enthalpies of combustion and formation of 5,12-dihydrotetracene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m$(cr) kJ mol^{-1}	$\Delta_f H^o_m$(cr) kJ mol^{-1}	Reference
1	na	i-SMB	mp: 211–212	5	no	m	-9190.0 ± 1.4	106.0 ± 2.7	1951MAG/HAR

Recommendation

$\Delta_f H^o_m$(cr, 298.15 K)	106.0 ± 2.7 kJ mol^{-1}	Available value	Entry 1

7.29.2. Enthalpy of fusion

Not available; T_{fus}: 481.2 K.

7.29.3. Enthalpy of vaporization

Not available.

7.29.4. Enthalpy of sublimation

TABLE 162. Sublimation enthalpy of 5,12-dihydrotetracene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	338–398	116	368	118.9	ME	na	1958HOY/PEP
2	na	120.5	na	na	na	na	1951MAG/BEC

[a]Sublimation enthalpies adjusted to T=298.15 K using Eq. (3) and an estimated heat for solid 5,12-dihydrotetracene of 275.2 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H^o_m$(298.15 K)	118.9 ± 1.0 kJ mol^{-1}	Available value	Entry 1

Evaluation

The uncertainty is associated with the temperature adjustment only.

7.29.5. Summary

TABLE 163. A summary of experimental and estimated phase change enthalpies of 5,12-dihydrotetracene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298 K)[a] kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K)+ $\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}
expt.				118.9	
estimated	26.1		87.4		113.5[a]

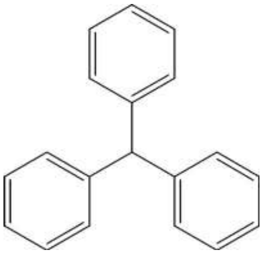
[a]Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})$=54.3 J mol^{-1} K^{-1}.

TABLE 164. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of 5,12-dihydrotetracene

$\Delta_f H_m^o$(cr, 298.15 K) kJ mol^{-1}	$\Delta_{sub} H_m^o$(298.15 K) kJ mol^{-1}	$\Delta_f H_m^o$(g, 298.15 K) kJ mol^{-1}
106.0 ± 2.7	118.9 ± 1.0[a]	224.9 ± 2.9

[a] The uncertainty is associated with the temperature adjustment only.

7.30. Triphenylmethane



Name	Formula	Registry Number	Molecular Weight
Triphenylmethane	$C_{19}H_{16}$	[519-73-3]	244.330 34 g mol^{-1}

7.30.1. Enthalpy of formation (solid)

TABLE 165. Standard enthalpies of combustion and formation of triphenylmethane at T = 298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs	Amount Reactn.	$\Delta_r H_m^o$(cr) kJ mol^{-1}	$\Delta_f H_m^o$(cr) kJ mol^{-1}	Reference
1	na	i-SMB	na	6	no	m	−9934.1 ± 2.7	170.8 ± 3.7	1970COX/PIL, 1947COO/MUL
2	na	i-SMB	na	9	no	m	−9925.9 ± 4.0	162.6 ± 4.7	1946PAR/WES
3	na	i-SMB	mp:93	10	na	m	−9988	225	1906SCH

Recommendation

$\Delta_f H_m^o$(cr, 298.15 K)	167.7 ± 4.1 kJ mol^{-1}	Suggested value	Entries 1 and 2

Evaluation

The suggested value has been calculated as the weighted average from the results of Coops *et al.* [1947COO/MUL] revised by Cox and Pilcher [1970COX/PIL] and Parks *et al.* [1946PAR/WES].

7.30.2. Enthalpy of fusion

TABLE 166. Fusion enthalpy of triphenylmethane

Entry	$\Delta_{fus} H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus} H_m^o$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	20.7 ± 0.4	367.2	16.0 ± 1.6	DSC	99.99	1999VER2
2	20.92	365.5	16.3	na	na	1944EIB
3	22.0	365.6	17.4	RC	na	1932SPA/THO
4	18.2 ± 1.4	365.5	13.6 ± 2.1	C	na	1917HIL/DUS

[a] Adjustment of the fusion enthalpy to T = 298.15 K using Eq. (5) and estimated heat capacities for liquid and solid triphenylmethane of 395.3 and 297 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$	20.7 ± 0.4 kJ mol^{-1}	Suggested value	Entry 1
$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$	16.0 ± 1.6 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.30.3. Enthalpy of vaporization

TABLE 167. Vaporization enthalpy of triphenylmethane

Entry	T_{Range} K	$\Delta_{\text{vap}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	298	93.7 ± 2.8	298	93.7 ± 2.8	CGC	99	1995HOS
2	343–462	$82.0\pm1.3^{\text{a}}$	403	$93.8\pm2.1^{\text{b}}$	EM	97.0	1989SAS/NGU
3	512–643	60.8	578	92.5^{b}	na	na	1987STE/MAL

[a] Uncertainty calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided in the reference.
[b] Vaporization enthalpy adjusted to $T=298.15$ K using Eq. (2) and an estimated heat capacity of 395.3 J mol^{-1} K^{-1} for liquid triphenylmethane.

Recommendation

$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$	93.8 ± 2.1 kJ mol^{-1}	Suggested value	Entries 1 and 2

Evaluation

The suggested value is the average of the first two entries.

7.30.4. Enthalpy of sublimation

TABLE 168. Sublimation enthalpy of triphenylmethane

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	323–353	106.7 ± 1.1	338	109.1 ± 1.3	GS	0.9999	1999VER2
2	343–363	$113.9\pm4.1^{\text{a}}$	353	$116.4\pm4.2^{\text{b}}$	EM	0.97	1989SAS/NGU
3	325–349	100.1^{c}	337	101.8^{b}	na	na	1987STE/MAL
4	303–358	106.8	331	$108.2\pm4.6^{\text{b}}$	GS	0.995+	1986HAN/ECK
5	326–349	100.1 ± 0.8	339	$101.9\pm1.0^{\text{b}}$	VG	na	1959AIH
6	299–364	100.8 ± 8.3	332	$102.2\pm8.3^{\text{b}}$	QF	na	1936CUT/BEN

[a] Calculated by a Clausius-Clapeyron treatment of the vapor pressure–temperature data provided.
[b] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid triphenylmethane of 297 J mol^{-1} K^{-1}.
[c] Calculated from the Antoine constants.

Recommendation

$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\text{ K})$	108.4 ± 2.8 kJ mol^{-1}	Suggested value	Entries 1 and 4

Evaluation

The suggested value is the mean of entries 1 and 4; the uncertainty represents an average uncertainty associated with the two entries. These two entries were selected on the basis how well Eq. (4) was satisfied; see below.

7.30.5. Summary

TABLE 169. A summary of experimental and estimated phase change enthalpies of triphenylmethane

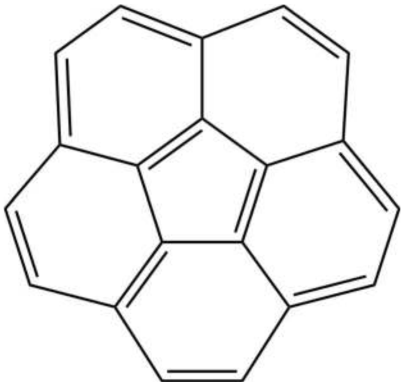
	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K)+\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}
expt.	20.7 ± 0.4	16.0 ± 1.6	93.8 ± 2.1	108.4 ± 0.3	109.8 ± 2.6
estimated	26.1		87.4		113.5[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=72.1\ J\ mol^{-1}\ K^{-1}$.

TABLE 170. A summary of suggested enthalpies of sublimation and formation in the condensed and gas phases of triphenylmethane

$\Delta_f H^o_m(cr, 298.15\ K)$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298.15\ K)$ kJ mol^{-1}	$\Delta_f H^o_m(g, 298.15\ K)$ kJ mol^{-1}
167.7 ± 4.1	108.4 ± 2.8	276.1 ± 5.0

7.31. Corannulene



Name	Formula	Registry Number	Molecular Weight
Corannulene	$C_{20}H_{10}$	[5821-51-2]	250.2934 g mol^{-1}

7.31.1. Enthalpy of formation (solid)

TABLE 171. Standard enthalpies of combustion and formation of corannulene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m$ (cr) kJ mol^{-1}	$\Delta_f H^o_m$(cr) kJ mol^{-1}	Reference
1	na	i-smb	^{1}H-nmr GC/MS HPLC	6	Electric heating	m	-9641.5 ± 5.4	$342.2 \pm [6.0]$	1995KIY/NAG

Recommendation

$\Delta_f H^o_m(cr, 298.15\ K)$	342.2 ± 6.0 kJ mol^{-1}	Available value	Entry 1

7.31.2. Enthalpy of fusion

TABLE 172. Fusion enthalpy of corannulene

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H_m^o(298\ K)$[a] kJ mol^{-1}	Method	Purity %	Reference
1	17.3 ± 1.2	542.3	0.8 ± 5.6	DSC	99+	2002CHI/WEB

[a]Fusion enthalpies adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid naphthalene of 374.5 and 263 J mol^{-1} K^{-1}, respectively; the difference of 0.3 kJ mol^{-1} from the literature value reflects a numerical error in the temperature adjustment.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	17.3 ± 1.2 kJ mol^{-1}	Available value	Entry 1
$\Delta_{fus}H_m^o(298.15\ K)$	0.8 ± 5.6 kJ mol^{-1}	Available value	Entry 1

7.31.3. Enthalpy of vaporization

TABLE 173. Vaporization enthalpy of corannulene

Entry	$\Delta_{vap}H_m(T)$ kJ mol^{-1}	T K	$\Delta_{vap}H_m^o(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	112.4 ± 1.9	298	112.4 ± 1.9	CGC	99+	2002CHI/WEB

Recommendation

$\Delta_{vap}H_m^o(298.15\ K)$	112.4 ± 1.9 kJ mol^{-1}	Available value	Entry 1

Evaluation

The value reported here differs from the value reported previously [2002CHI/WEB] in that it has been readjusted using updated vaporization enthalpies of the n-alkanes [2004CHI/HAN] used as standards in the evaluation of the vaporization enthalpy of corannulene.

7.31.4. Enthalpy of sublimation

TABLE 174. Sublimation enthalpy of corannulene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H_m^o(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	391–425	115.4 ± 8.0	408	119.4 ± 8.1[a]	HSA	99+	2002CHI/WEB

[a]Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid corannulene of 263 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H_m^o(298.15\ K)$	119.4 ± 8.1 kJ mol^{-1}	Available value	Entry 1

7.31.5. Summary

TABLE 175. A summary of experimental and estimated phase change enthalpies for corannulene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)+\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}
expt.	17.3 ± 1.2	0.8 ± 5.6	112.4 ± 1.9	119.4 ± 8.1	113.2 ± 5.9
estimated	17.9		96.8		114.7[a]

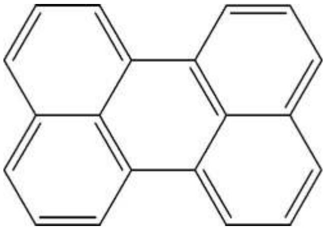
[a]Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=33$ J mol^{-1} K^{-1} (corannulene was estimated as a PAH and not as an unsaturated cyclopentane using the ring equation.

TABLE 176. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of corannulene

$\Delta_f H^o_m$(cr, 298.15 K)	$\Delta_{sub} H^o_m$(298.15 K)	$\Delta_f H^o_m$(g, 298.15 K)
kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
342.2 ± 6.0	116.3 ± 7.0[a]	458.5 ± 9.2

[a] Due to the large uncertainties associated with the sublimation enthalpies measured both directly and indirectly, the sublimation enthalpy used is the mean of the results obtained by both methods; the uncertainty represents two standard deviations of the mean.

7.32. Perylene



Name	Formula	Registry Number	Molecular Weight
Perylene	$C_{20}H_{12}$	[198-55-0]	252.309 28 g mol^{-1}

7.32.1. Enthalpy of formation (solid)

TABLE 177. Standard enthalpies of combustion and formation of perylene at T=298.15 K

	Purity			Num. of	Aux.	Amount	$\Delta_r H^o_m$(cr)	$\Delta_f H^o_m$(cr)	
Entry	%	Method	Charact.	exp.	Subs.	Reactn.	kJ mol^{-1}	kJ mol^{-1}	Reference
1	na	i-SMB	na	na	na	na	−9767.6 ± 0.5	182.4 ± [2.7]	1970COX/PIL, 1967WES/WON
2	na	i-SMB	na	10	no	m	−9772 ± 18	186 ± 18	1929PON/GRI

Recommendation

$\Delta_f H^o_m$(cr, 298.15 K)	182.4 ± 2.7 kJ mol^{-1}	Available value	Entry 1

Evaluation

The selected value is that given by Westrum and Wong [1967WES/WON] revised and recalculated by Cox and Pilcher [1970COX/PIL].

7.32.2. Enthalpy of fusion

TABLE 178. Fusion enthalpy of perylene

	$\Delta_{fus} H_m(T_{fus})$	T_{fus}	$\Delta_{fus} H^o_m$(298 K)[a]		Purity	
Entry	kJ mol^{-1}	K	kJ mol^{-1}	Method	%	Reference
1	32.58 ± 0.3	551.3	15.3 ± 5.7	DTA	99.89	1992SAB/ELW
2	31.76 ± 1.2	553.9	14.3 ± 5.8	DSC	purum[b]	1973CAS/VEC
3	31.87 ± 0.08	550.9	14.6 ± 5.7	AC	99.97	1971WON/WES

[a] Fusion enthalpy adjusted to T=298.15 K using Eq.(5) and estimated heat capacities for liquid and solid perylene of 385.4 and 279.2 J mol^{-1} K^{-1}, respectively.

[b] Fluka, AG, Buchs, Switerland.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	31.87 ± 0.08 kJ mol^{-1}	Recommended value	Entry 3
$\Delta_{fus}H_m^o(298.15\ K)$	14.6 ± 5.7 kJ mol^{-1}	Recommended value	Entry 3

Evaluation

Perylene has been recommended as a secondary standard for fusion enthalpy measurements [1992SAB/ELW]. The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.32.3. Enthalpy of vaporization

TABLE 179. Vaporization enthalpy of perylene

Entry	$\Delta_{vap}H_m(T)$ kJ mol^{-1}	T K	$\Delta_{vap}H_m^o(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	118.5 ± 1.2	298	118.5 ± 1.2	CGC	99.5	2008ZHA/UNH
2	na	na	89.9	GC	99	2002LEI/CHA

Recommendation

$\Delta_{vap}H_m^o(298.15\ K)$	118.5 ± 1.2 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

Entry 1 is chosen as the most probable value. Vaporization enthalpies reported by gas chromatography (entry 2) have given consistently lower than values reported by other techniques. The value of entry 1 reported here differs from the value reported previously in that it has been readjusted using updated vaporization enthalpies of the n-alkanes used as standards in the evaluation of the vaporization enthalpy of perylene.

7.32.4. Enthalpy of sublimation

TABLE 180. Sublimation enthalpy of perylene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H_m^o(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	390–432	126.2 ± 1.6	411	131 ± 2.3	ME	99+	2008GOL/SUU
2	397–415	132.6 ± 3.6	408	137.2 ± 4.5 [a]	ME	99.0+	1998OJA/SUU
3	313–453	123.2		na	GS	99.9	1995NAS/LEN
4	443–518	137.6 ± 2.5	481	144.8 ± 4.2	C	99.0+	1973GIG/MAL
5	443–518	137.9 ± 3.8	481	145.2 ± 5.0	ME	99.0+	1973GIG/MAL
6	383–453	139	418	144.1[a]	na	na	1958HOY/PEP
7	415	129.6 ± 2.1	415	134.6 ± 5.4 [a]	ME	mp[b]	1952INO/SHI

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid perylene of 279.2 J mol^{-1} K^{-1}.

[b] Characterized only by melting point: 534 K.

Recommendation

$\Delta_{sub}H_m^o(298.15\ K)$	135.9 ± 2.6 kJ mol^{-1}	Suggested value	Entries 2 and 7

Evaluation

The suggested value is the mean of entries 2 and 7. This selection is based on the agreement found in the sublimation enthalpy calculated from the sum of the vaporization and fusion enthalpies adjusted for temperature using the protocol outlined by Eqs. (2)–(5) (see below). The uncertainty represents two standard deviations of the mean. No experimental details are provided in 1995NAS/LEN.

7.32.5. Summary

TABLE 181. A summary of experimental and estimated phase change enthalpies for perylene

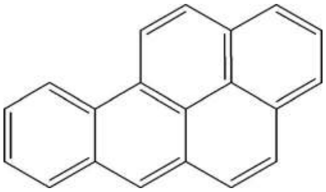
	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K)^{-1}$ kJ mol^{-1}	$\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K)+$ $\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}
expt.	31.87 ± 0.08	14.6 ± 5.7	118.5 ± 1.2	135.9 ± 2.6	133.1 ± 5.8
estimated	31.6		96.8		128.7[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=42.4$ J mol^{-1} K^{-1}.

TABLE 182. A summary of available enthalpies of sublimation and formation in the condensed and gas phase of perylene

$\Delta_f H^o_m(cr, 298.15\ K)$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298.15\ K)$ kJ mol^{-1}	$\Delta_f H^o_m(g, 298.15\ K)$ kJ mol^{-1}
182.4 ± 2.7	135.9 ± 2.6	318.3 ± 3.7

7.33. Benzo[*a*]pyrene



Name	Formula	Registry Number	Molecular Weight
Benzo[*a*]pyrene, 3,4-benzopyrene	$C_{20}H_{12}$	[50-32-8]	252.309 28 g mol^{-1}

7.33.1. Enthalpy of formation (solid)

None available.

7.33.2. Enthalpy of fusion

TABLE 183. Fusion enthalpy of benzo[*a*]pyrene

Entry	$\Delta_{trans}H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H^o_m(298\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1			16.5 ± 0.5	449.6	6.18[a]	na	98	1998RUZ/MOK
2			15.1	451	4.7[a]	DSC	98	1995HAI/SAN
3			17.4[b]	451[c]	7.0[a]	DSC	99+	1990HIN/BID
4	8.5 ± 0.2[d]	390	17.3 ± 0.6	454	6.7 ± 3.5[a]	DSC	99.0+	1973CAS/VEC

[a] Fusion enthalpy adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid benzo[*a*]pyrene of 385.4 and 279.2 J mol^{-1} K^{-1}, respectively.
[b] Calculated from the experimental entropy of fusion assuming $T_{fus}=451$ K.
[c] Assumed.
[d] An average of a broad transition from $T=383$ K to $T=396$ K.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$	17.3 ± 0.6 kJ mol^{-1}	Available value	Entry 4
$\Delta_{\mathrm{fus}}H^{\circ}_{\mathrm{m}}(298.15\ \mathrm{K})$	6.7 ± 3.5 kJ mol^{-1}	Available value	Entry 4
$\Delta_{\mathrm{tpce}}H^{\circ}_{\mathrm{m}}(298.15\ \mathrm{K})$	15.3 ± 3.5 kJ mol^{-1}	Available value	Entry 4

Evaluation

Casellato *et al.* [1973CAS/VEC] reported a broad transtion between $T=383$ K and $T=396$ K on samples not previously melted. Ruzicka *et al.* [1998RUZ/MOK] reported the heat capacity of benzo[*a*]pyrene from $T=307$ K to 407 K and did not report any anomalous behavior. They did comment on an unusually high degree of scatter in their data to which they attributed to impurities. They did not comment on the broad transition reported by Casellato *et al.* (entry 4). The data reported by Ruzicka *et al.* (entry 1) refer to the triple point temperature. It is possible that the two reports are measurements made on two polymorphic forms. The fusion enthalpy selected is the result reported in the fourth entry. The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment. No experimental details are reported in entries 2 and 3.

7.33.3. Enthalpy of vaporization

TABLE 184. Vaporization enthalpy of benzo[*a*]pyrene

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H^{\circ}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	298	118.4 ± 0.6	298	118.4 ± 0.6	CGC	97[a]	2008HAN/NUT
2	298	117.1 ± 3.2	298	117.1 ± 3.2	CGC	97[a]	2004CHI/HAN
3	na	na	na	105.0 ± 3.0	GC	98+	2006HAF/PAR
4	na	na	na	91	GC	99	2002LEI/CHA
5	452–462	97.0 ± 1.3[b]	457	114.5 ± 2.8[c]	PG	98	1998RUZ/MOK

[a] The chromatography generally separates any impurities.

[b] Calculated from the data provided.

[c] Calculated using Eq.(2) and an estimated heat capacity of liquid benzo[*a*]pyrene of 385.4 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{vap}}H^{\circ}_{\mathrm{m}}(298.15\ \mathrm{K})$	116.7 ± 2.3 kJ mol^{-1}	Available value	Entries 1, 2, 5

Evaluation

Ruzicka *et al.* [1998RUZ/MOK] recommended a vaporization enthalpy value of 97.1 kJ mol^{-1} at the triple point, $T=459$ K. However, their recommendations appear to be based on measurements only over a 10 K temperature range. The mean of entries 1, 2, and 5 is selected.

7.33.4. Enthalpy of sublimation

TABLE 185. Sublimation enthalpy of benzo[*a*]pyrene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\circ}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	392–424	113.3 ± 3.1	408	118.0 ± 3.5[a]	ME	99+	2008GOL/SUU
2	422–447	115.1 ± 2.0[b]	434	120.9 ± 2.8[a,c]	na	98	1998RUZ/MOK
3	313–453	122.5	na	na	GS	99.9	1995NAS/LEN
4	358–431	118.5[d]	395	122.6	na	na	1987STE/MAL
5	na	na	na	110.9	GC	na	1984YAM/KUW
6	358–431	118.3 ± 1.2	395	122.6 ± 1.8[a]	ME	96.3	1974MUR/POT

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid benzo[*a*]pyrene of 279.2 J mol^{-1} K^{-1}.

[b] Calculated from the data provided.

[c] The results cited by the authors include their own measurements and may include an evaluation of a previous literature value [1974MUR/POT].

[d] Calculated from the Antoine constants.

Recommendation

$\Delta_{sub}H^o_m$(298.15 K)	120.5 ± 2.7 kJ mol^{-1}	Available value	Entries 1, 2, 6

Evaluation

Ruzicka *et al.* recommended a sublimation enthalpy of 118.1 kJ mol^{-1} at T=298.15 K. Application of Eq. (3) to their results of 115.1 ± 2.0 kJ mol^{-1} at T=434 K provides the value of 120.9 ± 2.8 at T=298.15 K, cited as the second entry. Since the results in entry 6 were also adjusted with Eq. (3), for consistency, we have used the value estimated by this equation, 120.9 kJ mol^{-1} for this entry. The sublimation enthalpy cited below the table is the mean of entries 1, 2, and 6. Entries 4 and 6 probably refer to the same measurements; only entry 6 was used. Since all the vapor pressure measurements were reported near or above T=396 K, two values are cited in the recommendation of the sublimation enthalpy of benzopyrene at T=298 K because of the possibility of polymorphism (see the discussion below Table 183).

7.33.5. Summary

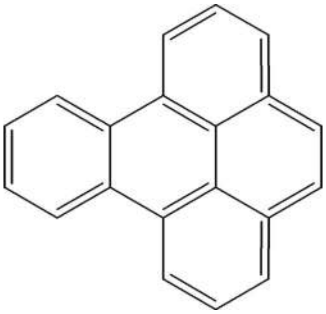
TABLE 186. A summary of experimental and estimated phase change enthalpies for benzo[*a*]pyrene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K)+ $\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}
expt.	17.3 ± 0.6	6.7 ± 3.5	116.7 ± 2.3	120.5 ± 2.7	123.4 ± 4.2[a]
		15.3 ± 3.5	116.7 ± 2.3	129.0 ± 2.7	132.0 ± 4.2[a]
estimated	19.2		96.8		116[b]

[a] Two values are cited because of the possibility of polymorphism; see the discussion below Tables 183 and 185.

[b] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})$=42.4 J mol^{-1} K^{-1}.

7.34. Benzo[*e*]pyrene



Name	Formula	Registry Number	Molecular Weight
Benzo[*e*]pyrene, 1,2-benzopyrene	$C_{20}H_{12}$	[192-97-2]	252.309 28 g mol^{-1}

7.34.1. Enthalpy of formation (solid)

None available.

7.34.2. Enthalpy of fusion

TABLE 187. Fusion enthalpy of benzo[*e*]pyrene

Entry	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	19.2[b]	454[c]	8.6	DSC	99+	1990HIN/BID
2	16.6 ± 0.8[d]	454	5.94 ± 3.5	DSC	na	1973CAS/VEC

[a] Total phase change enthalpy adjusted to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid benzo[*e*]pyrene of 385.4 and 279.2 J mol^{-1} K^{-1}, respectively.

[b] Calculated from the experimental entropy of fusion assuming T_{fus}=454 K.

[c] Assumed.

[d] The authors note that a crystal transition is observed from T=420 K to T=432 K and assigned an approximate transition enthalpy of 2.5 kJ mol^{-1}.

Recommendation

$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$	16.6 ± 0.8 kJ mol^{-1}	Available value	Entry 2
$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}$(298.15 K)	5.9 ± 3.5 kJ mol^{-1}	Available value	Entry 2
$\Delta_{\text{tpce}}H^{\text{o}}_{\text{m}}$(298.15 K)	8.4 ± 4.3 kJ mol^{-1}	Available value	Entry 2

Evaluation

The total phase change enthalpy was adjusted to T=298.15 K as noted above; the uncertainty in this value includes an estimate of the uncertainty associated with the temperature adjustment as well as the uncertainty associated with the transition enthalpy (±2.5 kJ mol^{-1}).

7.34.3. Enthalpy of vaporization

TABLE 188. Vaporization enthalpy of benzo[*e*]pyrene

Entry	$\Delta_{\text{vap}}H_{\text{m}}(T)$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	118.2 ± 0.6	298	118.2 ± 0.6	CGC	99	2008HAN/NUT
2	na	na	105 ± 3.0	GC	99.4	2006HAF/PAR
3	na	na	110.5	GC	na	1984YAM/KUW

Recommendation

$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}$(298 K)	118.2 ± 0.6 kJ mol^{-1}	Available value	Entry 1

Evaluation

Entry 1 when combined with $\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}$(298.15 K) gives the best value for $\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$(298.15 K).

7.34.4. Enthalpy of sublimation

TABLE 189. Sublimation enthalpy of benzo[*e*]pyrene

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	313–453	117.9	na	na	GS	99.9	1995NAS/LEN
2	359–423	119.1 ± 1.2	391	123.0 ± 1.8	ME	98.2	1974MUR/POT

[a] Sublimation enthalpies adjusted to T=298.15 K using Eq. (3) and an estimated heat capacity for solid benzo[*e*]pyrene of 279.2 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H_m^o(298.15\ K)$	123.0 ± 1.8 kJ mol^{-1}	Suggested value	Entry 2

Evaluation

The value from entry 1 was not used because there are not sufficient details reported about the measurements. The transition enthalpy is not added to the sublimation enthalpy at $T=298.15$ since it occurs above the temperature range of measurement.

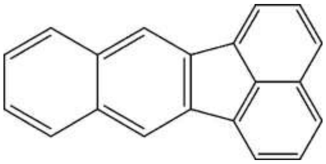
7.34.5. Summary

TABLE 190. A summary of experimental and estimated phase change enthalpies for benzo[*e*]pyrene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)+\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}
expt.	16.6 ± 0.8	8.4 ± 4.3	118.2 ± 0.6	123.0 ± 1.8	126.6 ± 4.3
estimated	19.2		96.8		116.0[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=42.4$ J mol^{-1} K^{-1}.

7.35. Benzo[*k*]fluoranthene



Name	Formula	Registry Number	Molecular Weight
Benzo[*k*]fluoranthene, 8,9-benzofluoranthene, 11,12-benzofluoranthene	$C_{20}H_{12}$	[207-08-9]	252.309 28 g mol^{-1}

7.35.1. Enthalpy of formation (solid)

TABLE 191. Standard enthalpies of combustion and formation of benzo[*k*]fluoranthene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_cH_m^o(cr)$ kJ mol^{-1}	$\Delta_fH_m^o(cr)$ kJ mol^{-1}	Reference
1	99+	i-SMB	ea HPLC	6	n-hexadecane	m	-9757.6 ± 3.4	172.4 ± 4.3	2002DIO/MIN

Recommendation

$\Delta_fH_m^o(cr, 298.15\ K)$	172.4 ± 4.3 kJ mol^{-1}	Highly questionable value	Entry 1

Evaluation

Theoretical calculations [2004YU/SUM, 2005SIV/TRA] suggest that the value by Diogo y Minas da Piedade is about 40 kJ mol^{-1} too low. Furthermore, the experimental enthalpy of formation in the gas phase of benzo[*k*]fluoranthene is only 4 kJ mol^{-1} higher than the enthalpy of formation of fluoranthene, which has one less benzene ring. By comparison, fluoranthene's $\Delta_fH_m^o(g)$ is in turn about 30 kJ mol^{-1} higher than the $\Delta_fH_m^o(g)$ of acenaphthylene, which has one benzene ring less than fluoranthene. Therefore, the experimental enthalpy of formation is highly questionable.

7.35.2. Enthalpy of fusion

TABLE 192. The fusion enthalpy of benzo[*k*]fluoranthene

Entry	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$[a] kJ mol^{-1}	Method	Purity %	Reference
1	27.5 ± 0.1	489.3	14.5 ± 4.3	DSC	99+	2002DIO/MIN

[a] Total phase change enthalpy adjusted to $T = 298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid benzo[*e*]pyrene of 384.7 and 278.6 J mol^{-1} K^{-1}, respectively.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$	27.5 ± 0.1 kJ mol^{-1}	Suggested value	Entry 1
$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	14.5 ± 4.3 kJ mol^{-1}	Suggested value	Entry 1

7.35.3. Enthalpy of vaporization

TABLE 193. Vaporization enthalpy of benzo[*k*]fluoranthene

Entry	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(T)$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	117.4 ± 2.2	298	117.4 ± 2.2	CGC	98[a]	2008HAN/NUT
2	na	na	105.5 ± 3.0	GC	98+	2006HAF/PAR
3	na	na	88.5	GC	na	2002LEI/CHA

[a] The chromatography generally separates any impurities.

Recommendation

$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	117.4 ± 2.2 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

Entry 1 when combined with $\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ gives the best value for $\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$.

7.35.4. Enthalpy of sublimation

TABLE 194. Sublimation enthalpy of benzo[*k*]fluoranthene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	387–424	127.8 ± 3.1	406	133.3 ± 4.5	ME	99+	2002DIO/MIN
2	389–468	130.0 ± 2.6	429	134.2	ME	90	1974MUR/POT

[a] Sublimation enthalpies adjusted to $T = 298.15$ K using Eq. (3) and an estimated heat capacity for solid benzo[*k*]fluoranthene of 278.6 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	133.8 ± 4.5 kJ mol^{-1}	Suggested value	Entries 1 and 2

Evaluation

The suggested value is the average of the two entries.

7.35.5. Summary

TABLE 195. A summary of experimental and estimated phase change enthalpies for benzo[*k*]fluoranthene

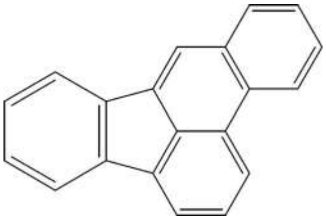
	$\Delta_{\rm fus}H_{\rm m}(T_{\rm fus})$ kJ mol^{-1}	$\Delta_{\rm fus}H^{\rm o}_{\rm m}$(298 K) kJ mol^{-1}	$\Delta_{\rm vap}H^{\rm o}_{\rm m}$(298 K) kJ mol^{-1}	$\Delta_{\rm sub}H^{\rm o}_{\rm m}$(298 K) kJ mol^{-1}	$\Delta_{\rm fus}H^{\rm o}_{\rm m}$(298 K)+ $\Delta_{\rm vap}H^{\rm o}_{\rm m}$(298 K) kJ mol^{-1}
expt.	27.5 ± 0.1	14.5 ± 4.3	117.4 ± 2.2	133.8 ± 4.5	131.9 ± 4.8
estimated	17.4		96.8		113.2[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\rm tpce}S(T_{\rm fus})=35.6$ J mol^{-1} K^{-1} (estimated as a PAH).

TABLE 196. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of benzo[*k*]fluoranthene

$\Delta_{\rm f}H^{\rm o}_{\rm m}$(cr, 298.15 K) kJ mol^{-1}	$\Delta_{\rm sub}H^{\rm o}_{\rm m}$(298.15 K) kJ mol^{-1}	$\Delta_{\rm f}H^{\rm o}_{\rm m}$(g, 298.15 K) kJ mol^{-1}
172.4 ± 4.3	133.8 ± 4.5	306.2 ± 6.2

7.36. Benz[*e*]acephenanthrylene



Name	Formula	Registry Number	Molecular Weight
Benz[*e*]acephenanthrylene, benz[*b*]fluoranthene, 3,4-benzofluoranthene, 2,3-benzofluoranthene	$C_{20}H_{12}$	[205-99-2]	252.309 28 g mol^{-1}

7.36.1. Enthalpy of formation (solid)

None available.

7.36.2. Enthalpy of fusion

None available; $T_{\rm fus}$: 437.2 K.

7.36.3. Enthalpy of vaporization

TABLE 197. Vaporization enthalpy of 2,3-benzofluoranthene

Entry	$\Delta_{\rm vap}H_{\rm m}(T)$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\rm vap}H^{\rm o}_{\rm m}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	116.8 ± 3.2	298	116.8 ± 3.2	CGC	99	2008HAN/NUT
2	na	na	104.0 ± 3.0	GC	98+	2006HAF/PAR
3	na	na	89.7	GC	na	2002LEI/CHA

Recommendation

$\Delta_{\rm vap}H^{\rm o}_{\rm m}$(298.15 K)	116.8 ± 3.2 kJ mol^{-1}	Questionable value	Entry 1

Evaluation

This value was chosen on the basis of the similarity of its magnitude to values measured for similar isomers (benzo[*k*]fluoranthene, benzo[*e*]pyrene, and benzo[*a*]pyrene).

7.36.4. Enthalpy of sublimation

Table 198. Sublimation enthalpy of 2,3-benzofluoranthene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	313–453	119.2	na	na	GS	99.9	1995NAS/LEN

Recommendation

$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	119.2 kJ mol^{-1}	Questionable value	Entry 1

Evaluation

No experimental details are provided in 1995NAS/LEN.

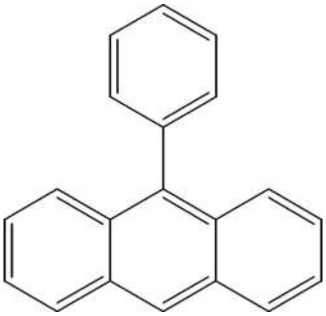
7.36.5. Summary

Table 199. A summary of experimental and estimated phase change enthalpies for 2,3-benzofluoranthene

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.			116.8 ± 3.2	119.2	
estimated	15.6		96.8		112.4[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=35.6$ J mol^{-1} K^{-1} (estimated as a PAH).

7.37. 9-Phenylanthracene



Name	Formula	Registry Number	Molecular Weight
9-Phenylanthracene	$C_{20}H_{14}$	[602-55-1]	254.325 16 g mol^{-1}

7.37.1. Enthalpy of formation (solid)

None available.

7.37.2. Enthalpy of fusion

Table 200. Fusion enthalpy of 9-phenylanthracene

Entry	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})^{\mathrm{a}}$ kJ mol^{-1}	Method	Purity %	Reference
1	25.5 ± 0.8	427.6	16.6 ± 3.0	DSC	na	1979FAR/SHA

[a] Adjustment of the fusion enthalpy to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid 9-phenylanthracene of 397 and 296 J T/K mol^{-1} K^{-1}.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	25.5 ± 0.8 kJ mol^{-1}	Suggested value	Entry 1
$\Delta_{fus}H^o_m(298.15\ K)$	16.6 ± 3.0 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The fusion enthalpy was adjusted to $T = 298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.37.3. Enthalpy of vaporization

TABLE 201. Vaporization enthalpy of 9-phenylanthracene

Entry	T_{Range} K	$\Delta_{vap}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H^o_m(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	91.6	GC	na	2002LEI/CHA
2	430–510	84.4[a]	470	104.0[b]	na	na	1987STE/MAL
3	435–465	86.3 ± 2.5[c]	450	103.6 ± 3.5	TE/HSA	na	1974SHI/GRE

[a] Calculated from the constant provided.
[b] Vaporization enthalpy adjusted to $T = 298.15$ K using Eq. (2) and an estimated heat capacity of 397 J mol^{-1} K^{-1} for liquid 9-phenylanthracene.
[c] The vaporization enthalpy was calculated from the vapor pressure equation obtained from the combined HSA and TE measurements over the temperature range specified in column 2 by a $\log p$ vs $1/T$ treatment.

Recommendation

$\Delta_{vap}H^o_m(298.15\ K)$	103.8 ± 3.5 kJ mol^{-1}	Suggested value	entries 2 and 3

Evaluation

The suggested value is the average of the second and third entries. Vaporization enthalpies reported by GC (entry 1) have been consistently lower than values reported by other techniques.

7.37.4. Enthalpy of sublimation

TABLE 202. Sublimation enthalpy of 9-phenylanthracene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	313–453	118.7	na	na	GS	99.9	1995NAS/LEN
2	430–510	115.2	470	123.0 ± 2.6[a,b]	na	na	1987STE/MAL
3	353–383	116.9 ± 1.2[c]	368	120.1 ± 1.6	TE/HSA	na	1974SHI/GRE
4	na	115.3	na	118.5	na	na	1958KLO

[a] Sublimation enthalpies adjusted to $T = 298.15$ K using Eq. (3) and an estimated heat capacity for solid 9-phenylanthracene of 296 J mol^{-1} K^{-1}.
[b] Uncertainty is due to the temperature adjustment.
[c] The sublimation enthalpy was calculated from the vapor pressure equation obtained from the combined HSA and TE measurements over the temperature range specified in column 2 by a $\log p$ vs $1/T$ treatment.

Recommendation

$\Delta_{sub}H^o_m(298.15\ K)$	120.5 ± 3.4 kJ mol^{-1}	Suggested value	Entries 2–4

Evaluation

The sublimation value is the mean of entries 2–4; the uncertainty represents two standard deviations of the mean and an average uncertainty associated with the temperature adjustment. There are no experimental details cited in 1995NAS/LEN.

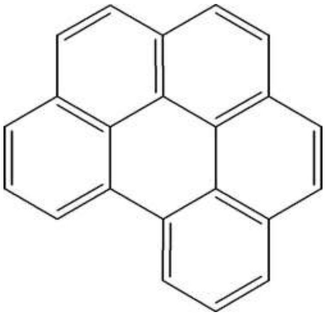
7.37.5. Summary

TABLE 203. A summary of phase change enthalpies for 9-phenylanthracene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K)+ $\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}
expt.	25.5 ± 0.8	16.6 ± 3.0	103.8 ± 3.5	120.5 ± 3.4	120.2 ± 4.6
estimated	25.1		96.8		121.9[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=58.6$ J mol^{-1} K^{-1}.

7.38. Benzo[*ghi*]perylene



Name	Formula	Registry Number	Molecular Weight
Benzo[*ghi*]perylene, 1,12-benzoperylene	$C_{22}H_{12}$	[191-24-2]	276.330 68 g mol^{-1}

7.38.1. Enthalpy of formation (solid)

None available.

7.38.2. Enthalpy of fusion

TABLE 204. Fusion enthalpy of benzo[*ghi*]perylene

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H^o_m$(298 K)^a kJ mol^{-1}	Method	Purity %	Reference
1	17.6 ± 0.2	553	na	DSC	na	1980SMI
2	17.4 ± 0.9	554	na	DSC	98.0+	1973CAS/VEC

Recommendation

$\Delta_{fus}H_m(T_{fus})$	17.5 ± 0.2 kJ mol^{-1}	Suggested value	Entry 1
$\Delta_{fus}H^o_m$(298.15 K)	−(1.3 ± 6.3) kJ mol^{-1}		

Evaluation

The suggested value is the mean of both entries. The uncertainty represents two standard deviations of the mean. Adjustment of the fusion enthalpy to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid benzo[*ghi*]perylene of 417.4 and 297.4 J mol^{-1} K^{-1} results in a negative fusion enthalpy. Equation (5) is not applicable over this temperature range for this compound. However, examination of the uncertainty suggests that the fusion enthalpy could be as large as +5.0 kJ mol^{-1}. Examination of Table 207 suggests a fusion enthalpy at $T=298.15$ K of approximately 4.0 kJ mol^{-1}.

7.38.3. Enthalpy of vaporization

TABLE 205. Vaporization enthalpy of benzo[*ghi*]perylene

Entry	$\Delta_{vap}H_m(T)$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H^o_m(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	128.9 ± 3.0	298	128.9 ± 3.0	CGC	98[a]	2008HAN/NUT
2	na	na	96.1	GC	na	2002LEI/CHA

[a] The chromatography generally separates any impurities.

Recommendation

$\Delta_{vap}H^o_m(298.15\ K)$	128.9 ± 3.0 kJ mol^{-1}	Available value	Entry 1

Evaluation

Vaporization enthalpies reported by GC (entry 2) have been consistently lower than values reported by other techniques.

7.38.4. Enthalpy of sublimation

TABLE 206. Sublimation enthalpy of benzo[*ghi*]perylene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	313–453	129.9	na	na	GS	99.9	1995NAS/LEN
2	389–468	127.8 ± 1.5	428	132.7 ± 2.2[a]	ME	94.6	1974MUR/POT
3	390–512	126.0	450[b]	133 ± 2.3[a]	ME	na	1967WAK/INO

[a] Sublimation enthalpies adjusted to $T = 298.15$ K using Eq. (3) and an estimated heat capacity for solid benzo[*ghi*]perylene of 279.4 J mol^{-1} K^{-1}.

[b] Mean temperature range approximate.

Recommendation

$\Delta_{sub}H^o_m(298.15\ K)$	132.9 ± 2.3 kJ mol^{-1}	Suggested value	entries 2 and 3

Evaluation

The suggested value is the mean of entries 2 and 3. The value from entry 1 was not used because there are not sufficient details reported about the measurements.

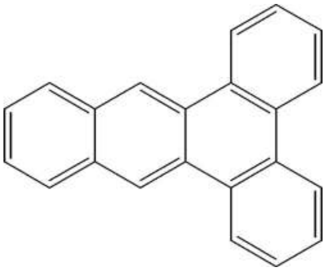
7.38.5. Summary

TABLE 207. A summary of experimental and estimated phase change enthalpies for benzo[*ghi*]perylene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K) + \Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}
expt.	17.5 ± 0.2	-1.3 ± 6.3	128.9 ± 3.0	132.9 ± 2.3	128.9 ± 7.0
estimated	22.7		106.2		128.9[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus}) = 41$ J mol^{-1} K^{-1}.

7.39. Benzo[*b*]triphenylene



Name	Formula	Registry Number	Molecular Weight
Benzo[*b*]triphenylene, 1,2:3,4-dibenzanthracene, dibenz[*a*,*c*]anthracene	$C_{22}H_{14}$	[215-58-7]	278.346 56 g mol^{-1}

7.39.1. Enthalpy of formation (solid)

TABLE 208. Standard enthalpies of combustion and formation of 1,2:3,4-dibenzanthracene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m(\mathrm{cr})$ kJ mol^{-1}	$\Delta_f H^o_m(\mathrm{cr})$ kJ mol^{-1}	Reference
1	99.94	i-smb	DSC	6	Benzoic acid	m	−10 842.8 ± 8.2	184.8 ± 8.7	1986YAM

Recommendation

$\Delta_f H^o_m(\mathrm{cr}, 298.15\ \mathrm{K})$	184.8 ± 8.7 kJ mol^{-1}	Available value	Entry 1

7.39.2. Enthalpy of fusion

TABLE 209. Fusion enthalpy of 1,2:3,4-dibenzanthracene

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H^o_m(298\ \mathrm{K})$[a] kJ mol^{-1}	Method	Purity %	Reference
1	25.8 ± 0.07	553.5	6.9 ± 6.2	DSC	puriss[b]	1973CAS/VEC

[a] Fusion enthalpy adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid benzo[*b*]triphenylene of 427.6 and 313 J mol^{-1} K^{-1}, respectively.

[b] Koch-Light Laboratory, Colnbrook, UK.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	25.8 ± 0.1 kJ mol^{-1}	Available value	Entry 1
$\Delta_{fus}H^o_m(298\ \mathrm{K})$	6.9 ± 6.2 kJ mol^{-1}	Available value	Entry 1

Evaluation

The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.39.3. Enthalpy of vaporization

TABLE 210. Vaporization enthalpy of 1,2:3,4-dibenzanthracene

Entry	$\Delta_{vap}H_m(T)$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H^o_m(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	132.3 ± 1.8	298.15	132.3 ± 3.6	CGC	99+	2004CHI/HAN
2	na	na	97.5	GC	99+	2002LEI/CHA

Recommendation

$\Delta_{vap}H^o_m(298.15\ K)$	132.3 ± 3.6 kJ mol^{-1}	Available value	Entry 1

Evaluation

Vaporization enthalpies reported by GC (entry 2) have been consistently lower than values reported by other techniques.

7.39.4. Enthalpy of sublimation

TABLE 211. Sublimation enthalpy of 1,2:3,4-dibenzanthracene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	313–453	135	na	na	GS	99.9	1995NAS/LEN
2	425–452	139.1 ± 4	440	159 ± 6.0[a]	TE, ME	97.0+	1980DEK

[a] A temperature adjustment of just under 20 kJ mol^{-1} seems high; the sublimation enthalpy adjusted to $T = 298.15$ K using Eq. (3) and an estimated heat capacity for solid benzo[*b*]triphenylene of 313 J mol^{-1} K^{-1} result in an adjustment of only 6.7 kJ mol^{-1} and a sublimation enthalpy of 145.9 kJ mol^{-1}.

Recommendation

$\Delta_{sub}H^o_m(298.15\ K)$	145.9 ± 6.0 kJ mol^{-1}	Available value	Entry 2

Evaluation

There is no supporting experimental information in 1995NAS/LEN; it is not clear whether the results reported in this work refer to $T = 298.15$ K. The value of 145.9 ± 6.0 kJ mol^{-1} (see footnote a, Table 211) is selected because of the better agreement found between the sublimation, fusion, and vaporization enthalpies; see Table 212 below.

7.39.5. Summary

TABLE 212. A summary of experimental and estimated phase change enthalpies for 1,2:3,4-dibenzanthracene

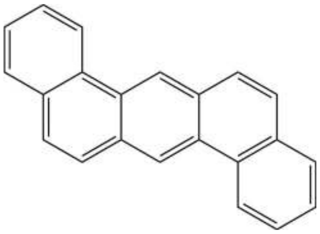
	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K) +$ $\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}
expt.	$25.8 \pm .0.1$	6.9 ± 6.2	132.3 ± 3.6	145.9 ± 6.0	139.2 ± 7.2
estimated	24.1		106.2		130.3[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus}) = 43.6$ J mol^{-1} K^{-1}.

TABLE 213. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of benzo[*b*]triphenylene

$\Delta_fH^o_m(cr, 298.15\ K)$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298.15\ K)$ kJ mol^{-1}	$\Delta_fH^o_m(g, 298.15\ K)$ kJ mol^{-1}
184.8 ± 8.7	145.9 ± 6.0	330.7 ± 10.6

7.40. Dibenz[*a*, *h*]anthracene



Name	Formula	Registry Number	Molecular Weight
Dibenz[*a*,*h*]anthracene 1,2:5,6-dibenzanthracene	$C_{22}H_{14}$	[53-70-3]	278.346 56 g mol^{-1}

7.40.1. Enthalpy of formation (solid)

TABLE 214. Standard enthalpies of combustion and formation of 1,2:5,6-dibenzanthracene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m(\text{cr})$ kJ mol^{-1}	$\Delta_f H^o_m(\text{cr})$ kJ mol^{-1}	Reference
1	99.61	i-smb	DSC	6	Benzoic acid	m	$-108\,36.8 \pm 9.8$	$178.8 \pm [10.2]$	1986YAM

Recommendation

$\Delta_f H^o_m(\text{cr}, 298.15\text{ K})$	178.8 ± 10.2 kJ mol^{-1}	Available value	Entry 1

7.40.2. Enthalpy of fusion

TABLE 215. Fusion enthalpy of 1,2:5,6-dibenzanthracene

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H^o_m(298\text{ K})^a$ kJ mol^{-1}	Method	Purity %	Reference
1	31.17 ± 1.0	544.2	13.0 ± 6.1	DSC	puriss[b]	1973CAS/VEC

[a] Fusion enthalpy adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid 1,2:5,6-dibenzanthracene of 427.6 and 313 J mol^{-1} K^{-1}, respectively.

[b] Koch-Light Laboratories, Colnbrook, UK.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	31.2 ± 1.0 kJ mol^{-1}	Suggested value	Entry 1
$\Delta_{fus}H^o_m(298.15\text{ K})$	13.0 ± 6.1 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean $(\pm 2\sigma)$ as well as an estimate of the uncertainty associated with the temperature adjustment.

7.40.3. Enthalpy of vaporization

TABLE 216. Vaporization enthalpy of 1,2:5,6-dibenzanthracene

Entry	$\Delta_{vap}H_m(T)$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H^o_m(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	131.1 ± 1.4	298.15	131.1 ± 2.8	CGC	99+	2004CHI/HAN
2	na	na	99.4	GC	99+	2002LEI/CHA

Recommendation

$\Delta_{vap}H^o_m(298.15\text{ K})$	131.1 ± 2.8 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

Vaporization enthalpies reported by GC (entry 2) have been consistently lower than values reported by other techniques.

7.40.4. Enthalpy of sublimation

TABLE 217. Sublimation enthalpy of 1,2:5,6-dibenzanthracene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	313–453	134.1	na	na	GS	99.9	1995NAS/LEN
2	436–462	141.6 ± 4	449.5	162 ± 6[a]	TE,ME	98	1980DEK
3	403–512	142.0	458[b]	149.0 ± 2.3[c]	ME	na	1967WAK/INO

[a] A temperature adjustment of 20 kJ mol^{-1} seems high; the sublimation enthalpy adjusted to T = 298.15 K using Eq. (3) and an estimated heat capacity for solid 1,2:5,6-dibenzanthracene of 313 J mol^{-1} K^{-1} result in a temperature adjustment of 7.2 kJ mol^{-1} and a sublimation enthalpy of 148.8 ± 6 kJ mol^{-1}..

[b] The mean temperature is approximate.

[c] Sublimation enthalpies adjusted to T = 298.15 K using Eq. (3) and an estimated heat capacity for solid 1,2:5,6-dibenzanthracene of 313 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K)	148.9 ± 4.2 kJ mol^{-1}	Suggested value	Entries 2 and 3

Evaluation

The value is the mean of entries 2 (see footnote a in Table 217) and 3. The value of 148.9 ± 4.2 kJ mol^{-1} is selected because of the agreement found between the sublimation, fusion, and vaporization enthalpies; see below. The uncertainty at T = 298.15 K is an average value. There are no experimental details cited in 1995NAS/LEN.

7.40.5. Summary

TABLE 218. A summary of experimental and estimated phase change enthalpies for 1,2:5,6-dibenzanthracene

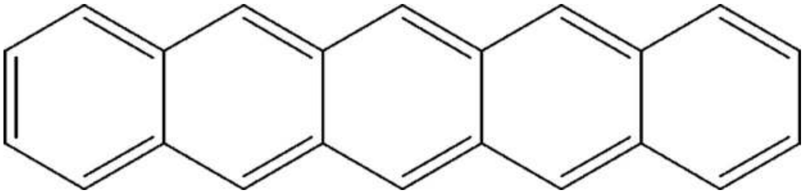
	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}$(298 K) kJ mol^{-1}	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$(298 K) kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$(298 K) kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}$(298 K) + $\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$(298 K) kJ mol^{-1}
expt.	31.2 ± 1.0	13.0 ± 6.1	131.1 ± 2.8	148.9 ± 4.2	144.1 ± 6.7
estimated	23.7		106.2		129.9[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})$ = 43.6 J mol^{-1} K^{-1}.

TABLE 219. A summary of available enthalpies of sublimation and formation in the condensed and gas phases, of 1,2:5,6-dibenzanthracene

$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}$(cr, 298.15 K) kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K) kJ mol^{-1}	$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}$(g, 298.15 K) kJ mol^{-1}
178.8 ± 10.2	148.9 ± 4.2	328 ± 11

7.41. Pentacene



Name	Formula	Registry Number	Molecular Weight
Pentacene	$C_{22}H_{14}$	[135-48-8]	278.346 56 g mol^{-1}

7.41.1. Enthalpy of formation (solid)

None available.

7.41.2. Enthalpy of fusion

None available.

7.41.3. Enthalpy of vaporization

None available.

7.41.4. Enthalpy of sublimation

TABLE 220. Sublimation enthalpy of pentacene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	443–483	156.9 ± 13.6	463	164.8 ± 13.8[a]	ME	98	1998OJA/SUU
2	495–530	154 ± 10.0	513	184 ± 20[b]	TE, ME	F[c]	1980DEK
3	444–555	158.1	500[d]	167.6 ± 3.2[a]	ME	na	1967WAK/INO

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid pentacene of 313 J mol^{-1} K^{-1}.
[b] A temperature adjustment of 30 kJ mol^{-1} seems excessive; the sublimation enthalpy adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid pentacene of 313 J mol^{-1} K^{-1} result in a temperature adjustment of 7.2 kJ mol^{-1} and a sublimation enthalpy of 164.2 ± 10.5 kJ mol^{-1}.
[c] Fluka Chemical Co.
[d] Temperature range approximate.

Recommendation

$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$	165.5 ± 12.3 kJ mol^{-1}	Available value	Entries 1–3

Evaluation

The suggested value is the mean of all entries adjusted to $T=298.15$ K using Eq. (3) (see footnote a, Table 220); the uncertainty represents two standard deviations of the mean as well as the contribution to the temperature adjustment.

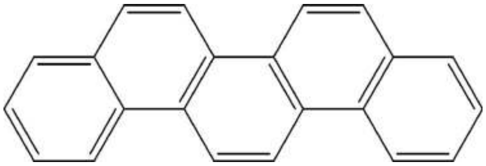
7.41.5. Summary

TABLE 221. A summary of experimental and estimated phase change enthalpies for pentacene

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.				165.5 ± 12.3	
estimated	na[a]		106.2		

[a] Melting point not available.

7.42. Picene



Name	Formula	Registry Number	Molecular Weight
Picene	$C_{22}H_{14}$	[213-46-7]	278.346 56 g mol^{-1}

7.42.1. Enthalpy of formation (solid)

None available.

7.42.2. Enthalpy of fusion

TABLE 222. Fusion enthalpy of picene

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H^o_m(298\text{ K})$[a] kJ mol^{-1}	Method	Purity %	Reference
1	35.2 ± 0.8	637	10.1 ± 8.3[a]	DSC	95	1973CAS/VEC

[a] Fusion enthalpy adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid picene of 427.6 and 313 J mol^{-1}K^{-1}, respectively.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	35.2 ± 0.8 kJ mol^{-1}	Available value	Entry 1
$\Delta_{fus}H^o_m(298.15\text{ K})$	10.1 ± 8.3 kJ mol^{-1}	Available value	Entry 1

Evaluation

The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.42.3. Enthalpy of vaporization

None available.

7.42.4. Enthalpy of sublimation

TABLE 223. Sublimation enthalpy of picene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m(298.15\text{ K})$ kJ mol^{-1}	Method	Purity %	Reference
1	413–555	140.7	480[a]	149.4 ± 2.9[b]	ME	na	1967WAK/INO

[a] Temperature range approximate.

[b] Sublimation enthalpy adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid picene of 313 J mol^{-1}K^{-1}.

Recommendation

$\Delta_{sub}H^o_m(298.15\text{ K})$	149.4 ± 2.9 kJ mol^{-1}	Available value	Entry 1

Evaluation

The uncertainty cited is associated only with the temperature adjustment.

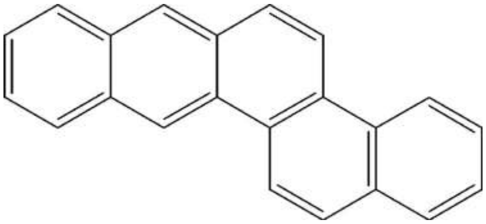
7.42.5. Summary

TABLE 224. A summary of experimental and estimated phase change enthalpies for picene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\text{ K})$ kJ mol^{-1}	$\Delta_{vap}H^o_m(298\text{ K})$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298\text{ K})$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\text{ K})+\Delta_{vap}H^o_m(298\text{ K})$ kJ mol^{-1}
expt.	35.2 ± 0.8	10.1 ± 8.3		149.4 ± 2.9	
estimated	27.8		106.2		134.0[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=43.6$ J mol^{-1}K^{-1}.

7.43. 1,2:6,7-Dibenzophenanthrene



Name	Formula	Registry Number	Molecular Weight
1,2:6,7-Dibenzophenanthrene, benz(*b*)chrysene	$C_{22}H_{14}$	[214-17-5]	278.346 56 g mol^{-1}

7.43.1. Enthalpy of formation (solid)

None available.

7.43.2. Enthalpy of fusion

None available; T_{fus}: 565 K [1987STE/MAL].

7.43.3. Enthalpy of vaporization

None available.

7.43.4. Enthalpy of sublimation

TABLE 225. Sublimation enthalpy of 1,2:6,7-dibenzophenanthrene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	398–513	136.9	456	144.4[a]	na	na	1987STE/MAL

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat for solid 1,2:6,7-dibenzophenanthrene of 313 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	144.4 ± 2.5 kJ mol^{-1}	Available value	Entry 1

Evaluation

The uncertainty represents that only associated with the temperature adjustment.

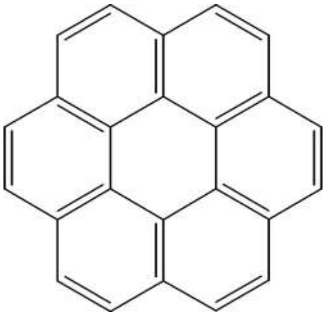
7.43.5. Summary

TABLE 226. A summary of experimental and estimated phase change enthalpies for 1,2:6,7-dibenzophenanthrene

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.				144.4 ± 2.5	
estimated	24.6		106.2		130.8[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=43.6$ J mol^{-1} K^{-1}.

7.44. Coronene



Name	Formula	Registry Number	Molecular Weight
Coronene	$C_{24}H_{12}$	[191-07-1]	300.352 08 g mol^{-1}

7.44.1. Enthalpy of formation (solid)

TABLE 227. Standard enthalpies of combustion and formation of coronene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m$(cr) kJ mol^{-1}	$\Delta_f H^o_m$(cr) kJ mol^{-1}	Reference
1	na	i-smb	^{1}H-nmr	3	vaseline	m	−11 305.7 ± 3.6	146.2 ± 4.8	2000NAG
2	99.7+	i-smb	^{1}H-nmr	7	Electric heating	m	−11 311.5 ± 6.1	152.3 ± 6.9	1995KIY

Recommendation

$\Delta_f H^o_m$(cr, 298.15 K)	152.3 ± 6.9 kJ mol^{-1}	Available value	Entry 2

7.44.2. Enthalpy of fusion

TABLE 228. Fusion enthalpy of coronene

Entry	$\Delta_{trans} H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus} H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{tpce} H^o_m$(298 K) kJ mol^{-1}	Method	Purity %	Reference
1	0.44 ± 0.24	225				AC	99+	1980WON/WES
2			19.2 ± 2.4	710.5		DSC	na	1980SMI

Recommendation

$\Delta_{fus} H^o_m(T_{fus})$	19.2 ± 2.4 kJ mol^{-1}	Available value	Entry 1
$\Delta_{tcpe} H_m(T_{fus})$	19.6 ± 2.4 kJ mol^{-1}	Available value	Entry 1 plus 2
$\Delta_{tcpe} H^o_m$(298.15 K)	none available		

Evaluation

The uncertainty includes the standard deviation of the mean ($\pm 2\sigma$). Adjustment of the fusion enthalpy to T=298.15 K using Eq. (5) using estimated heat capacities for liquid and solid coronene of 449.4 and 315.6 J mol^{-1} K^{-1} respectively, results in a negative fusion enthalpy; Eq. (5) is not applicable over this temperature range.

7.44.3. Enthalpy of vaporization

TABLE 229. Vaporization enthalpy of coronene

Entry	$\Delta_{\rm vap}H_{\rm m}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\rm vap}H^{\rm o}_{\rm m}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	139.5 ± 3.0	298	139.5 ± 6.0	CGC	99[a]	2008CHI, 2002CHI/WEB
2	na	na	104.2	GC	99+	2002LEI/CHA

[a] Not relevant to the measurement; the chromatography generally separates any impurities; vaporization enthalpy is determined by gas chromatography as a mixture.

Recommendation

$\Delta_{\rm vap}H^{\rm o}_{\rm m}$(298.15 K)	139.5 ± 6.0 kJ mol^{-1}	Available value	Entry 1

Evaluation

The value reported here differs from the value reported previously [2002CHI/WEB] in that it has been readjusted using updated vaporization enthalpies of the n-alkanes used as standards in the evaluation of the vaporization enthalpy of coronene. Vaporization enthalpies reported by GC (entry 2) have been consistently lower than values reported by other techniques.

7.44.4. Enthalpy of sublimation

TABLE 230. Sublimation enthalpy of coronene

Entry	$T_{\rm Range}$ K	$\Delta_{\rm sub}H_{\rm m}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\rm sub}H^{\rm o}_{\rm m}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	421–504	133.1 ± 10.2	463	141.0 ± 10.5[a]	ME	na	1998OJA/SUU
2	313–453	143.2	na	na	GS	99.9	1995NAS/LEN
3	427–510	135.9 ± 6.3	469	144.1 ± 6.9	ME	98.6	1974MUR/POT
4	422–555	129.0	488[b]	138.5	ME	na	1967WAK/INO
5	433–513	146.9	473	155.4		na	1958HOY/PEP
6	407	149.4	407	154.7[a]	ME	na	1952INO/SHI

[a] Sublimation enthalpy adjusted to T=298.15 K using Eq. (3) and an estimated heat capacity for solid coronene of 315.6 J mol^{-1} K^{-1}.
[b] Temperature range approximate.

Recommendation

$\Delta_{\rm sub}H^{\rm o}_{\rm m}$(298.15 K)	142.6 ± 8.7 kJ mol^{-1}	Available value	Entries 1 and 3

Evaluation

The sublimation enthalpy of coronene should exceed the vaporization enthalpy by at least a few kJ mol^{-1}. Taking into consideration the standard deviation associated with the measured vaporization enthalpy, this suggests that this value should at least exceed 139 kJ mol^{-1}. Averaging entries 1 and 3 results in a sublimation enthalpy of 142.6 ± 8.7 kJ mol^{-1}. There are no experimental details cited in 1995NAS/LEN.

7.44.5. Summary

TABLE 231. A summary of experimental and estimated phase change enthalpies for coronene

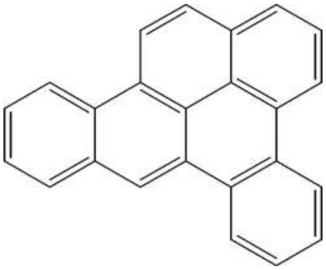
	$\Delta_{\rm fus}H_{\rm m}(T_{\rm fus})$ kJ mol^{-1}	$\Delta_{\rm fus}H^{\rm o}_{\rm m}$(298 K) kJ mol^{-1}	$\Delta_{\rm vap}H^{\rm o}_{\rm m}$(298 K) kJ mol^{-1}	$\Delta_{\rm sub}H^{\rm o}_{\rm m}$(298 K) kJ mol^{-1}	$\Delta_{\rm fus}H^{\rm o}_{\rm m}$(298 K) + $\Delta_{\rm vap}H^{\rm o}_{\rm m}$(298 K) kJ mol^{-1}
expt.	19.6 ± 2.4		139.5 ± 6.0	142.6 ± 8.7	>139; <158
estimated	28.1		115.6		143.7[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\rm tpce}S(T_{\rm fus})$=39.6 J mol^{-1} K^{-1}.

TABLE 232. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of coronene

$\Delta_f H_m^o$(cr, 298.15 K)	$\Delta_{sub} H_m^o$(298.15 K)	$\Delta_f H_m^o$(g, 298.15 K)
kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
152.3 ± 6.9	142.6 ± 8.7	294.9 ± 11.1

7.45. 1,2:4,5-Dibenzopyrene



Name	Formula	Registry Number	Molecular Weight
1,2:4,5-Dibenzopyrene, dibenzo[*a*,*e*]pyrene	$C_{24}H_{14}$	[192-65-4]	302.367 96 g mol^{-1}

7.45.1. Enthalpy of formation (solid)

None available.

7.45.2. Enthalpy of fusion

TABLE 233. Fusion enthalpy of 1,2:4,5-dibenzopyrene

Entry	$\Delta_{fus} H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus} H_m^o$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	30.5 ± 1.1	520.2	12.8 ± 5.9	DSC	puriss[b]	1973CAS/VEC

[a] Adjustment of the fusion enthalpy to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid 1,2:4,5-dibenzopyrene of 459.6 and 331.2 J mol^{-1} K^{-1}.

[b] Koch-Light Laboratries Colnbrook, England.

Recommendation

$\Delta_{fus} H_m(T_{fus})$	30.5 ± 1.1 kJ mol^{-1}	Available value	Entry 1
$\Delta_{fus} H_m^o$(298.15 K)	12.8 ± 5.9 kJ mol^{-1}	Available value	Entry 1

Evaluation

The fusion enthalpy was adjusted to T=298.15 K as noted above; the uncertainty in this value includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.45.3. Enthalpy of vaporization

None available.

7.45.4. Enthalpy of sublimation

TABLE 234. Sublimation enthalpy of 1,2:4,5-dibenzopyrene

Entry	T_{Range} K	$\Delta_{sub} H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub} H_m^o$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	413–526	146.5	470[a]	155.2[b]	ME	na	1967WAK/INO

[a] Temperature range approximate.

[b] Sublimation enthalpies adjusted to T=298.15 K using Eq. (3) and an estimated heat capacity for solid 1,2:4,5-dibenzopyrene of 331.2 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H^o_m$ (298.15 K)	155.2 kJ mol^{-1}	Available value	Entry 1

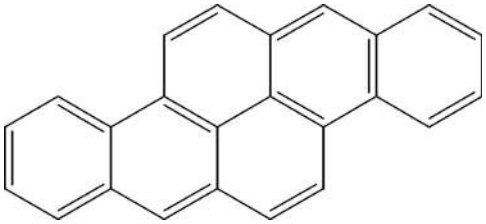
7.45.5. Summary

TABLE 235. A summary of experimental and estimated phase change enthalpies for 1,2:4,5-dibenzopyrene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K)+ $\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}
expt.	30.5 ± 1.0	12.8 ± 5.9		155.2	
estimated	22.0		115.6		137.6[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=42.2$ J mol^{-1} K^{-1}.

7.46. Dibenzo[*b*,*def*]chrysene



Name	Formula	Registry Number	Molecular Weight
Dibenzo[*b*,*def*]chrysene, dibenzo[*a*,*h*]pyrene, 3,4:8,9-dibenzopyrene, anthanthrene	$C_{24}H_{14}$	[189-64-0]	302.367 96 g mol^{-1}

7.46.1. Enthalpy of formation (solid)

None available.

7.46.2. Enthalpy of fusion

None available; T_{fus}: 537 K.

7.46.3. Enthalpy of vaporization

None available.

7.46.4. Enthalpy of sublimation

TABLE 236. Sublimation enthalpy of dibenzo[*b*,*def*]chrysene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	479	135.1	479	144.3[a]	ME	na[b]	1952INO/SHI

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid dibenzo[*b*,*def*]chrysene of 331.2 J mol^{-1} K^{-1}.
[b] Not available.

Recommendation

$\Delta_{sub}H^o_m$(298.15 K)	144.3 kJ mol^{-1}	Available value	Entry 1

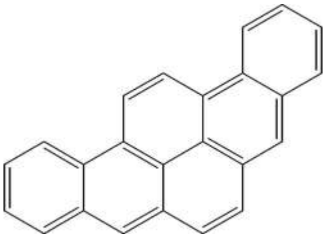
7.46.5. Summary

TABLE 237. A summary of experimental and estimated phase change enthalpies for dibenzo[*b*,*def*]chrysene

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.				144.3	
estimated	22.7		115.6		138.3[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=42.2$ J mol^{-1} K^{-1}.

7.47. Benzo[*rst*]pentaphene



Name	Formula	Registry Number	Molecular Weight
Benzo[*rst*]pentaphene, 3,4:9,10-dibenzopyrene, dibenzo[*a*,*i*]pyrene	$C_{24}H_{14}$	[189-55-9]	302.367 96 g mol^{-1}

7.47.1. Enthalpy of formation (solid)

None available.

7.47.2. Enthalpy of fusion

TABLE 238. Fusion enthalpy of benzo[*rst*]pentaphene

Entry	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$[a] kJ mol^{-1}	Method	Purity %	Reference
1	27.9 ± 1.2	556.8	7.3 ± 6.9	DSC	puriss[b]	1973CAS/VEC

[a] Adjustment of the fusion enthalpy to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid benzo[*rst*]pentaphene of 459.6 and 331.2 J mol^{-1} K^{-1}.

[b] Koch-Light Laboratories Ltd., Colnbrook, UK.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$	27.9 ± 1.2 kJ mol^{-1}	Available value	Entry 1
$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$	7.3 ± 6.9 kJ mol^{-1}	Available value	Entry 1

Evaluation

The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the measurement ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.47.3. Enthalpy of vaporization

None available.

7.47.4. Enthalpy of sublimation

None available.

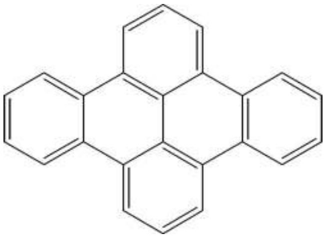
7.47.5. Summary

TABLE 239. A summary of experimental and estimated phase change enthalpies for dibenzo[*rst*]pentaphene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K)+ $\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}
expt.	27.9 ± 1.2	7.3 ± 6.9			
estimated	23.5		115.6		139.1

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=42.2$ J mol^{-1} K^{-1}.

7.48. Dibenzo[*fg*,*op*]naphthacene



Name	Formula	Registry Number	Molecular Weight
Dibenzo[*fg*,*op*]naphthacene, 1,2:6,7-dibenzpyrene, dibenzo[*e*]pyrene	$C_{24}H_{14}$	[192-51-8]	302.367 96 g mol^{-1}

7.48.1. Enthalpy of formation (solid)

None available.

7.48.2. Enthalpy of fusion

None available; T_{fus}: 624 K [1987STE/MAL].

7.48.3. Enthalpy of vaporization

None available.

7.48.4. Enthalpy of sublimation

TABLE 240. Sublimation enthalpy of dibenzo[*fg*,*op*]naphthacene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	430–555	147.4	492	157.2	ME	na	1987STE/MAL,1967WAK/INO

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid dibenzo[*fg*,*op*]naphthacene of 331.2 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H^o_m$(298.15 K)	157.2 kJ mol^{-1}	Available value	Entry 1

7.48.5. Summary

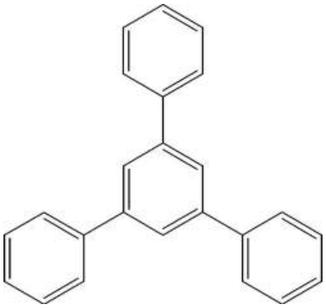
TABLE 241. A summary of experimental and estimated phase change enthalpies for dibenzo[*fg*,*op*]naphthacene

	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\text{ K})+\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\text{ K})$ kJ mol^{-1}
expt.				157.2	
estimated	25.9		115.6		141.5[b]

[a] Temperature of measurement; not known.

[b] The sum of the estimated fusion and vaporization enthalpy; estimated $\Delta_{\text{tpce}}S(T_{\text{fus}})=42.2$ J mol^{-1} K^{-1}.

7.49. 1,3,5-Triphenylbenzene



Name	Formula	Registry Number	Molecular Weight
1,3,5-Triphenylbenzene	$C_{24}H_{18}$	[612-71-5]	306.399 72 g mol^{-1}

7.49.1. Enthalpy of formation (solid)

TABLE 242. Standard enthalpies of combustion and formation of 1,3,5-triphenylbenzene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_{\text{r}}H^{\text{o}}_{\text{m}}(\text{cr})$ kJ mol^{-1}	$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}(\text{cr})$ kJ mol^{-1}	Reference
1	na	a-SMB	ea, mp	na	Benzoic acid	CO_2	−12 236.0 ± 5.4	218.8 ± [5.7]	1999KIP/LEB
2	99.99+	SMB	glc, DSC	5	oil	m	−12 238.7 ± 1.2	222.0 ± [3.4]	1997VER
3	na	SMB	na	12	no	m	−12 241.3 ± 5.3	224.6 ± [6.3]	1970COX/PIL, 1939RIC/PAR

Recommendation

$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}(\text{cr},298.15\text{ K})$	222.0 ± 3.4 kJ mol^{-1}	Suggested value	Entry 2

Evaluation

The suggested value is the one given by Verevkin [1997VER], and it is in the mean value of the three available data.

7.49.2. Enthalpy of fusion

TABLE 243. Fusion enthalpy of 1,3,5-triphenylbenzene

Entry	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\text{ K})$[a] kJ mol^{-1}	Method	Purity %	Reference
1	31.1 ± 1.0	448	19.0 ± 4.1	DSC	99.6	2004CHI/HAN
2	32.6 ± 0.4	445.2	20.7 ± 4.0	DSC	99.99	1997VER
3	33.4	446	21.5 ± 4.0	na	na	1982LEB/BYK
4	22.9 ± 0.6	448.5	10.7 ± 4.0	na	99.0+	1974MAL/BAR

[a] Fusion enthalpy adjusted to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid 1,3,5-triphenylbenzene of 484.2 and 366 J mol^{-1} K^{-1}, respectively.

Recommendation

$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$	32.4 ± 1.3 kJ mol^{-1}	Suggested value	Entries 1–3
$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K)	20.4 ± 4.0 kJ mol^{-1}	Suggested value	Entries 1–3

Evaluation

Fusion enthalpies reported for 1,3,5-triphenylbenzene are not totally in mutual agreement. The fusion enthalpy measured at the melting point is the mean of entries 1–3; the uncertainty represents two standard deviations of the mean. The fusion enthalpy was adjusted to T=298.15 K as noted above; the uncertainty includes the standard deviation of the mean ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.49.3. Enthalpy of vaporization

TABLE 244. Vaporization enthalpy of 1,3,5-triphenylbenzene

Entry	T_{Range} K	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	298	133.4 ± 2.0	298	133.4 ± 4.0	CGC[a]	99.6	2004CHI/HAN
2	454–500	116.6 ± 2.3	477	141.0 ± 3.7[b]	ME	99	1974MAL/BAR
3	454–500	119.5 ± 1.5	477	139.9 ± 2.8[b]	C	99	1974MAL/BAR

[a] Correlation-gas chromatography.

[b] Vaporization enthalpy adjusted to T=298.15 K using Eq. and an estimated heat capacity of 484 J mol^{-1} K^{-1} for liquid 1,3,5-triphenylbenzene.

Recommendation

$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K)	133.4 ± 4.0 kJ mol^{-1}	Suggested value	Entry 1

Evaluation

The value previously reported in 1998CHI/HES, 142.4 kJ mol^{-1}, has been adjusted using recent evaluations of the vaporization enthalpies of the n-alkane standards [1995HOS, 1994RUZ/MAJ, 2004CHI/HAN]; this value has been chosen on the basis that this value combined with $\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}$ (298.15 K) most closely reproduces the suggested sublimation enthalpies reported in Table 246; The fusion enthalpy reported above in Table 243 by the same workers of entries 2 and 3 also seems in error [1974MAL/BAR].

7.49.4. Enthalpy of sublimation

TABLE 245. Sublimation enthalpy of 1,3,5-triphenylbenzene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	407–429	141.2 ± 1.4	418	147.8 ± 1.4	ME	99.7	2006RIB/MON
2	364–388	145.6 ± 1.8	376	150.3 ± 1.8	GS	99.99	1997VER
3	410–444	142.1 ± 2.9	427	149.2 ± 7.7	ME	99	1974MAL/BAR
4	410–444	143.1 ± 0.6	427	150.3 ± 7.2	C	99	1974MAL/BAR
5	370–449	142.6	410[a]	148.8[b]	ME	na[c]	1967WAK/INO
6	363–408	143.6	386	148.5[b]	ME	na[c]	1958HOY/PEP

[a] This is the mean temperature cited by 1974MAL/BAR.

[b] Sublimation enthalpy adjusted to T=298.15 K using Eq. (3) and an estimated heat capacity for solid 1,3,5-triphenylbenzene of 366 J mol^{-1} K^{-1}.

[c] An independent analysis of composition other than a physical property such as melting point is not available.

Recommendation

$\Delta_{sub}H^o_m(298.15\ K)$	149.8 ± 1.6 kJ mol^{-1}	Recommended value	1999SAB/XU

Evaluation

1,3,5-Triphenylbenzene has been previously recommended as a tertiary standard for sublimation enthalpy measurements primarily because of the consistency of the sublimation enthalpy values reported for a compound of this size and volatility [1999SAB/XU]. The mean of these six runs is 149.2 ± 0.8 kJ mol^{-1}. The recommended value is retained.

7.49.5. Summary

TABLE 246. A summary of experimental and estimated phase change enthalpies for 1,3,5-triphenylbenzene

	$\Delta_{fus}H_m(T_{fus})$	$\Delta_{fus}H^o_m(298\ K)$	$\Delta_{vap}H^o_m(298\ K)$	$\Delta_{sub}H^o_m(298\ K)$	$\Delta_{fus}H^o_m(298\ K)+\Delta_{vap}H^o_m(298\ K)$
	kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
expt.	32.4 ± 1.3	20.4 ± 4.0	133.4 ± 4.0	149.8 ± 1.6	153.8 ± 5.7
estimated	39.4		115.6		155.0[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=88.2$ J mol^{-1} K^{-1}.

TABLE 247. A summary of suggested enthalpies of sublimation and formation in the condensed and gas phases of 1,3,5-triphenylbenzene

$\Delta_f H^o_m(cr, 298.15\ K)$	$\Delta_{sub}H^o_m(298.15\ K)$	$\Delta_f H^o_m(g, 298.15\ K)$
kJ mol^{-1}	kJ mol^{-1}	kJ mol^{-1}
222.0 ± 3.4	149.8 ± 1.6	371.8 ± 3.8

7.50. *p*-Quaterphenyl

Name	Formula	Registry Number	Molecular Weight
p-Quaterphenyl	$C_{24}H_{18}$	[135-70-6]	306.399 72 g mol^{-1}

7.50.1. Enthalpy of formation (solid)

TABLE 248. Standard enthalpies of combustion and formation of *p*-quaterphenyl at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m(cr)$ kJ mol^{-1}	$\Delta_f H^o_m(cr)$ kJ mol^{-1}	Reference
1	99.91	i-smb	DSC	6	no	m	$-12\,203.3 \pm 4.7$	186.6 ± 5.7	1986YAM
2	na	i-SMB	mp: 320–321 °C	6	na	na	$-12\,244 \pm 6$	227 ± 7	2005AFE/LIE, 1977BAL/LEB

Recommendation

$\Delta_f H^o_m(cr, 298.15\ K)$	227 ± 7 kJ mol^{-1}	Available value	Entry 2

Evaluation

The selected value is the one reported by Balepin *et al.* [1977BAL/LEB]. The selection of this value is based on the best agreement with the enthalpies of formation in the condensed state of benzene, biphenyl, and *p*-terphenyl as a function of the number of phenyl rings.

7.50.2. Enthalpy of fusion

TABLE 249. Fusion enthalpy of *p*-quaterphenyl

Entry	$\Delta_{trans}H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{tpce}H_m^o(298\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	1.1	190–260	57.6 ± 0.9	586.7	36.4 ± 7.8	DSC	zr[b]	1982WAS/RAD
2	1.0	450–540	37.8 ± 2.2	587.2	14.4 ± 8.0	DSC	na	1979SMI

[a] Total phase change enthalpy adjusted to $T=298.15$ K using Eq.(5) and estimated heat capacities for liquid and solid *p*-quaterphenyl of 484.2 and 366 J mol^{-1} K^{-1}, respectively.
[b] Zone refined.

Recommendation

$\Delta_{fus}H_m^o(587.0\ K)$	57.6 ± 0.9 kJ mol^{-1}	Available value	Entry 1
$\Delta_{tpce}H_m^o(298.15\ K)$	36.4 ± 7.8 kJ mol^{-1}	Available value	Entry 1

Evaluation

The fusion enthalpy was adjusted to $T=298.15$ K as noted above; the uncertainty in this value includes the standard deviation of the measurements ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment. The two measurements are in disagreement with each other. It should be noted that the results for biphenyl and *p*-terphenyl (Tables 51 and 144) by the authors of the first entry are higher than values by other workers. However, this value was chosen because it compares favorably with the value estimated for the fusion enthalpy of this material (see Table 251 below).

7.50.3. Enthalpy of vaporization

TABLE 250. Vaporization enthalpy of *p*-quaterphenyl

Entry	$\Delta_{vap}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H_m^o(298.15\ K)$ kJ mol^{-1}	Method	Purity %	Reference
1	133.4 ± 2.0	298	136.1 ± 3.2	CGC[a]	99.6	2008HAN/NUT

[a] Correlation-gas chromatography.

Recommendation

$\Delta_{vap}H_m^o(298.15\ K)$	136.1 ± 3.2 kJ mol^{-1}	Available value	Entry 1

7.50.4. Enthalpy of sublimation

None available.

Evaluation

An enthalpy of sublimation at $T=298.15$ K of 168.4 ± 1.6 kJ mol^{-1} has been measured by Ribeiro da Silva *et al.* [private communication, 2008RIB/SAN]. However, this result has yet to be published and is not analyzed further.

7.50.5. Summary

TABLE 251. A summary of experimental and estimated phase change enthalpies for *p*-quaterphenyl

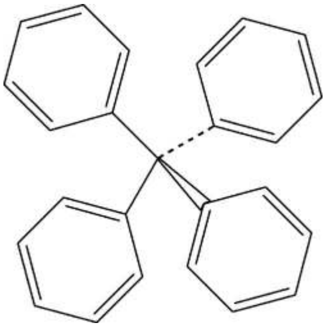
	$\Delta_{tpce}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{tpce}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H_m^o(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\ K)+\Delta_{vap}H_m^o(298\ K)$ kJ mol^{-1}
expt.	57.6 ± 0.9	36.4 ± 7.8	136.1 ± 3.2		172.5 ± 8.4
estimated	51.8		115.6		167.4[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=42.2$ J mol^{-1} K^{-1}.

TABLE 252. A summary of enthalpies of sublimation and formation in the condensed and gas phases of *p*-quaterphenyl

$\Delta_f H^o_m$(cr, 298.15 K) kJ mol^{-1}	$\Delta_{sub} H^o_m$(298.15 K) kJ mol^{-1}	$\Delta_f H^o_m$(g, 298.15 K) kJ mol^{-1}
227 ± 7	172.5 ± 8.4	400 ± 11

7.51. Tetraphenylmethane



Name	Formula	Registry Number	Molecular Weight
Tetraphenylmethane	$C_{25}H_{20}$	[630-76-2]	320.4263 g mol^{-1}

7.51.1. Enthalpy of formation (solid)

TABLE 253. Standard enthalpies of combustion and formation of tetraphenylmethane at T=298.15 K

Entry	Purity %	Method	Charact.	Num of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m$(cr) kJ mol^{-1}	$\Delta_f H^o_m$(cr) kJ mol^{-1}	Reference
1	na	SMB	na	9		m	−12 943.2 ± 2.5	247.2 ± [4.1]	1970COX/PIL, 1947COO/MUL, 1946COO/MUL
2	na	SMB	na	na	na	na	−13 000	300	2005AFE/LIE, 1934WIE/HEY
3	na	SMB	na	na	na	na	−12 988	292	2005AFE/LIE, 1906SCH

Recommendation

$\Delta_f H^o_m$(cr, 298.15 K)	247.2 ± 4.1 kJ mol^{-1}	Available value	Entry 1

7.51.2. Enthalpy of fusion

TABLE 254. Fusion enthalpy of tetraphenylmethane

Entry	$\Delta_{fus} H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus} H^o_m$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	48.28 ± 0.21	554.2	26.3 ± 7.3	DSC	99.99	1999VER2

[a] Adjustment of the fusion enthalpy to T=298.15 K using Eq. (5) and estimated heat capacities for liquid and solid tetraphenylmethane of 511.2 and 379 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{fus} H_m(T_{fus})$	48.3 ± 0.2 kJ mol^{-1}	Available value	Entry 1
$\Delta_{fus} H^o_m$(298.15 K)	26.3 ± 7.3 kJ mol^{-1}	Available value	Entry 1

7.51.3. Enthalpy of vaporization

None available.

7.51.4. Property

TABLE 255. Sublimation enthalpy of tetraphenylmethane

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	362–389	135.4 ± 2.6	375.8	140 ± 2.6	T	99.99	1999VER2
2	404–466	143.3	435	151.2[a]	na	na	1987STE/MAL
3	396–466	140.8 ± 5.0	431	150.6 ± 5.6[a]	ME	99+	1972KAN

[a] Sublimation enthalpies adjusted to T=298.15 K using Eq. 1.2 and an estimated heat capacity for solid tetraphenylmethan of 379 J K mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	140 ± 2.6 kJ mol^{-1}	Available value	1st entry

Evaluation

Two of the three values for tetraphenylmethane are in good agreement. However, it is not clear that the results listed in entry 2 are an independent measurement. The most recent value is selected because of the agreement observed between this value, the reported fusion enthalpy, and recent unpublished vaporization enthalpy measurements [2008LIP/CHI].

7.51.5. Summary

TABLE 256. A summary of experimental and estimated phase change enthalpies for tetraphenylmethane

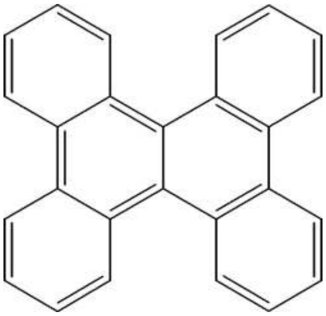
	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.	48.28 ± 0.21	26.3 ± 7.3		140.0 ± 2.6	
estimated	41.5		116.9		158.4[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})$=74.8 J mol^{-1} K^{-1}.

TABLE 257. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of tetraphenylmethane

$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{cr},298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{g},298.15\ \mathrm{K})$ kJ mol^{-1}
247.2 ± 4.1	140.0 ± 2.6	387.2 ± 4.9

7.52. Tetrabenzonaphthalene



Name	Formula	Registry Number	Molecular Weight
Tetrabenzonaphthalene, dibenzo[g,p]chrysene	$C_{26}H_{16}$	[191-68-4]	328.405 24 g mol^{-1}

7.52.1. Enthalpy of formation (solid)

TABLE 258. Standard enthalpies of combustion and formation of tetrabenzonaphthalene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H_m^o$(cr) kJ mol^{-1}	$\Delta_f H_m^o$(cr) kJ mol^{-1}	Reference
1	na	i-SMB	mp: 490 K	na	na	m	−12 897 ± 37	379 ± 37	1971WIT/BAR

Recommendation

$\Delta_f H_m^o$(cr, 298.15 K)	379 ± 37 kJ mol^{-1}	Available value	Entry 1

7.52.2. Enthalpy of fusion

None available; T_{fus}: 488 K.

7.52.3. Enthalpy of vaporization

None available.

7.52.4. Enthalpy of sublimation

TABLE 259. Sublimation enthalpy of tetrabenzonaphthalene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H_m^o$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	408–493	142.2	458^a	150.9^b	ME	na	1987STE/MAL,1967WAK/INO

[a] Temperature range obtained from 1987STE/MAL.

[b] Sublimation enthalpies adjusted to T=298.15 K using Eq. (3) and an estimated heat capacity for solid tetrabenzonaphthalene of 365 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H_m^o$(298.15 K)	150.9 kJ mol^{-1}	Available value	Entry 1

7.52.5. Summary

TABLE 260. A summary of experimental and estimated phase change enthalpies for tetrabenzonaphthalene

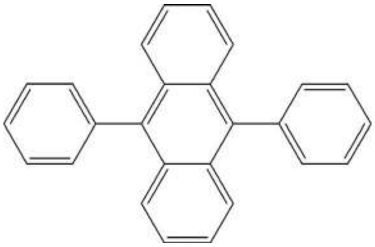
	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H_m^o$(298 K) kJ mol^{-1}	$\Delta_{vap}H_m^o$(298 K) kJ mol^{-1}	$\Delta_{sub}H_m^o$(298 K) kJ mol^{-1}	$\Delta_{fus}H_m^o$(298 K)+ $\Delta_{vap}H_m^o$(298 K) kJ mol^{-1}
expt.				150.9	
estimated	21.2		124.9		146.1^a

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})$=42.2 J mol^{-1} K^{-1}.

TABLE 261. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of tetrabenzonaphthalene

$\Delta_f H_m^o$(cr, 298.15 K) kJ mol^{-1}	$\Delta_{sub}H_m^o$(298.15 K) kJ mol^{-1}	$\Delta_f H_m^o$(g, 298.15 K) kJ mol^{-1}
379 ± 37	150.9	530

7.53. 9,10-Diphenylanthracene



Name	Formula	Registry Number	Molecular Weight
9,10-Diphenylanthracene	$C_{26}H_{18}$	[1499-10-1]	330.421 12 g mol^{-1}

7.53.1. Enthalpy of formation (solid)

TABLE 262. Standard enthalpies of combustion and formation of 9,10-diphenylanthracene at T=298.15 K

Entry	Purity %	Method	Charact	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_r H^o_m$(cr) kJ mol^{-1}	$\Delta_f H^o_m$(cr) kJ mol^{-1}	Reference
1	na	SMB	na	4	na	m	−13 112.4 ± 2.9	308.7 ± [4.5]	1970COX/PIL,1951MAG/HAR

Recommendation

$\Delta_f H^o_m$(cr, 298.15 K)	308.7 ± 4.5 kJ mol^{-1}	Available value	Entry 1

Evaluation

The available experimental value, given by Magnus *et al.* [1951MAG/HAR], was analyzed and recalculated by Cox and Pilcher [1970COX/PIL].

7.53.2. Enthalpy of fusion

None available; T_{fus}: 521 K.

7.53.3. Enthalpy of vaporization

TABLE 263. Vaporization enthalpy of 9,10-diphenylanthracene

Entry	T_{Range} K	$\Delta_{vap}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{vap}H^o_m$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	na	na	na	102.7	GC	99	2002LEI/CHA

Recommendation

$\Delta_{vap}H^o_m$(298.15 K)	102.7 kJ mol^{-1}	Questionable value	entry 1

Evaluation

Vaporization enthalpies reported by GC have been consistently lower than values reported by other techniques.

7.53.4. Enthalpy of sublimation

TABLE 264. Sublimation enthalpy of 9,10-diphenylanthracene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	313–453	137.5	na	na	GS	99.9	1995NAS/LEN
2	488	115.3	488	127.8[a]	AM	na	1958KLO

TABLE 264. Sublimation enthalpy of 9,10-diphenylanthracene—Continued

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
3	393–433	143.6	413	151.7[a]	na	na	1958HOY/PEP
4	481–502	156.9 ± 4.2	492	169.6 ± 5.9[a]	HSA	na	1953STE
5	na	133.9	na	na	na	na	1951MAG/BEC

[a] Sublimation enthalpy adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid 9,10-diphenylanthracene of 383 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$ (298.15 K)	169.6 ± 5.9 kJ mol^{-1}	Available value	Entry 4

Evaluation

The experimental value, entry 4, was chosen on the basis of the agreement between experiment and estimation *(vide infra)*. There are no experimental details cited in 1995NAS/LEN.

7.53.5. Summary

TABLE 265. A summary of experimental and estimated phase change enthalpies for 9,10-diphenylanthracene

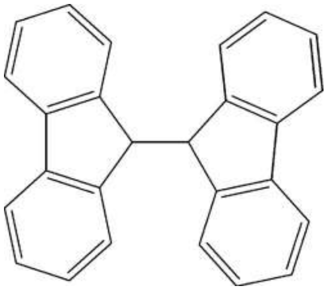
	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.				169.6 ± 5.9	
estimated	38.2		124.9		163.1[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=73.2$ J mol^{-1} K^{-1}.

TABLE 266. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of 9,10-diphenylanthracene

$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}(\mathrm{cr},298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}(\mathrm{g},298.15\ \mathrm{K})$ kJ mol^{-1}
308.7 ± 4.5	169.6 ± 5.9	478.3 ± 7.4

7.54. 9,9′-Bifluorenyl



Name	Formula	Registry Number	Molecular Weight
9,9′-Bifluorenyl, 9,9′-bi-9H-fluorene, 9,9′-bifluorene	$C_{26}H_{18}$	[1530-12-7]	330.421 12 g mol^{-1}

7.54.1. Enthalpy of formation (solid)

TABLE 267. Standard enthalpies of combustion and formation of 9,9′-bifluorenyl at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_c H_m^o$(cr) kJ mol^{-1}	$\Delta_f H_m^o$(cr) kJ mol^{-1}	Reference
1	>99.99	i-SMB	GC, DSC	6	oil	m	$-13\,001.2 \pm 0.8$	$197.5 \pm [3.5]$	1994RAK/VER

Recommendation

$\Delta_f H_m^o$ (cr, 298.15 K)	197.5 ± 3.5 kJ mol^{-1}	Available value	Entry 1

7.54.2. Enthalpy of fusion

TABLE 268. Fusion enthalpy of 9,9′-bifluorenyl

Entry	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{fus}H_m^o$(298 K)[a] kJ mol^{-1}	Method	Purity %	Reference
1	36.9	518	17.7 ± 6.3	DSC	99.99	1994RAK/VER

[a] Adjustment of the fusion enthalpy to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid 9,9′ bifluorenyl of 512.4 and 371.4 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{fus}H_m(T_{fus})$	36.9 kJ mol^{-1}	Available value	Entry 1
$\Delta_{fus}H_m^o$ (298.15 K)	17.7 ± 6.3 kJ mol^{-1}[a]	Available value	

[a] The uncertainty is due to the temperature adjustment.

7.54.3. Enthalpy of vaporization

None available.

7.54.4. Enthalpy of sublimation

TABLE 269. Sublimation enthalpy of 9,9′-bifluorenyl

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H_m^o$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	383–408	131.8 ± 2.3	395	132.6 ± 2.3	GS	99.9	1994RAK/VER

Recommendation

$\Delta_{sub}H_m^o$ (298.15 K)	132.6 ± 2.3 kJ mol^{-1}	Questionable temperature adjustment	Entry 1

Evaluation

Adjustment of the sublimation enthalpy to $T=298.15$ K using Eq. (3) and estimated heat capacities for solid 9,9′ bifluorenyl of 371.4 J mol^{-1} K^{-1} results in a value of 138.7 ± 3.2 kJ mol^{-1}. This value is in better agreement with the estimated value.

7.54.5. Summary

TABLE 270. A summary of experimental and estimated phase change enthalpies for 9,9′-bifluorenyl

	$\Delta_{\text{fus}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\ \text{K})$ kJ mol^{-1}	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\ \text{K})$ kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298\ \text{K})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\ \text{K})+\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\ \text{K})$ kJ mol^{-1}
expt.	36.9	17.7 ± 6.3		132.6 ± 2.3 (138.7 ± 3.2)[a]	
estimated	37.4		124.9		162.3[b]

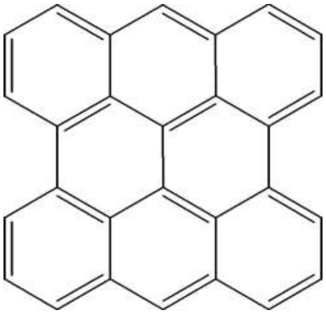
[a] This value was obtained by adjusting the sublimation enthalpy using Eq. (3).

[b] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\text{tpce}}S(T_{\text{fus}})=42.2$ J mol^{-1} K^{-1} (use of the ring equation)

TABLE 271. A summary of available enthalpies of sublimation and formation in the condensed and gas phases of 9,9′-bifluorenyl

$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}(\text{cr}, 298.15\ \text{K})$ kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\ \text{K})$ kJ mol^{-1}	$\Delta_{\text{f}}H^{\text{o}}_{\text{m}}(\text{g}, 298.15\ \text{K})$ kJ mol^{-1}
197.5 ± 3.5	132.6 ± 2.3	330.1 ± 4.2

7.55. *meso*-Naphthodianthrene



Name	Formula	Registry Number	Molecular Weight
meso-Naphthodianthrene, phenanthro[1,9,10,8-*fghij*]perylene	$C_{28}H_{14}$	[190-39-6]	350.410 76 g mol^{-1}

7.55.1. Enthalpy of formation (solid)

None available.

7.55.2. Enthalpy of fusion

None available.

7.55.3. Enthalpy of vaporization

None available.

7.55.4. Enthalpy of sublimation

TABLE 272. Sublimation enthalpy of *meso*-naphthodianthrene

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\ \text{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	580–630	180.5 ± 10	605	197.6 ± 11.5[a]	ME	na	1987STE/MAL, 1952INO/SHI

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid *meso*-naphthodianthrene of 367.6 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H_m^o$ (298.15 K)	197.6 ± 11.5 kJ mol^{-1}	Available value	Entry 1

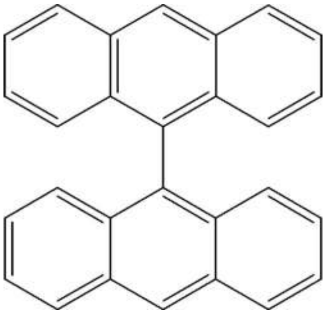
7.55.5. Summary

TABLE 273. A summary of experimental and estimated phase change enthalpies for *meso*-naphthodianthrene

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H_m^o$(298 K) kJ mol^{-1}	$\Delta_{vap}H_m^o$(298 K) kJ mol^{-1}	$\Delta_{sub}H_m^o$(298 K) kJ mol^{-1}	$\Delta_{fus}H_m^o$(298 K)+ $\Delta_{vap}H_m^o$(298 K) kJ mol^{-1}
expt.				197.6 ± 11.5	
estimated	na[a]		134.3		

[a] Melting point not available.

7.56. 9,9′-Bianthracene



Name	Formula	Registry Number	Molecular Weight
9,9′-Bianthracene	$C_{28}H_{18}$	[1055-23-8]	354.442 52 g mol^{-1}

7.56.1. Enthalpy of formation (solid)

TABLE 274. Standard enthalpies of combustion and formation of 9,9′-bianthracene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_cH_m^o$(cr) kJ mol^{-1}	$\Delta_fH_m^o$(cr) kJ mol^{-1}	Reference
1	na	SMB	m	5	no	m	−13916.9 ± 3.1	326.2 ± [4.8]	1970COX/PIL,1951MAG/HAR

Recommendation

$\Delta_fH_m^o$ (cr,298.15 K)	326.9 ± 4.8 kJ mol^{-1}	Available value	Entry 1

Evaluation

The value given by Magnus *et al.* [1951MAG/HAR] was analyzed and recalculated by Cox and Pilcher [1970COX/PIL].

7.56.2. Enthalpy of fusion

None available; T_{fus}: >633.2 K [1987STE/MAL].

7.56.3. Enthalpy of vaporization

None available.

7.56.4. Enthalpy of sublimation

TABLE 275. Sublimation enthalpy of 9,9′-bianthracene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	413–473	127.9	443	136.7^{a}	na	na	1987STE/MAL, 1958HOY/PEP
2	na	148	na	na	na	na	1951MAG/BEC

^{a}Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat for solid 9,9′-bianthracene of 400 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}$ (298.15 K)	148 kJ mol^{-1}	Questionable value	Entry 2

Evaluation

The value cited in entry 2 seems most probable. However, there are no details available (see the value estimated in Table 276).

7.56.5. Summary

TABLE 276. A summary of experimental and estimated phase change enthalpies for 9,9′-bianthracene

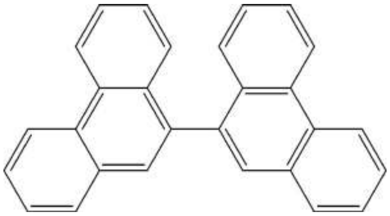
	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+$ $\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.				148	
estimated	>36.9		134.3		>171.2

^{a}Melting point T_{fus}: >633.2 K [1987STE/MAL]; $\Delta_{\mathrm{fus}}S_{\mathrm{m}}(T_{\mathrm{fus}})=58.2$ J mol^{-1} K^{-1} (estimated).

TABLE 277. A summary of available enthalpy of sublimation and formation in the gas phase of 9,9′-bianthracene

$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{cr}, 298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{g}, 298.15\ \mathrm{K})$ kJ mol^{-1}
326.9 ± 4.8	148	475

7.57. 9,9′-Biphenanthrene



Name	Formula	Registry Number	Molecular Weight
9,9′-Biphenanthrene	$C_{28}H_{18}$	[20532-03-0]	354.442 52 g mol^{-1}

7.57.1. Enthalpy of formation (solid)

TABLE 278. Standard enthalpies of combustion and formation of 9,9′-biphenanthrene at $T=298.15$ K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_{\mathrm{r}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{cr})$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H_{\mathrm{m}}^{\mathrm{o}}(\mathrm{cr})$ kJ mol^{-1}	Reference
1	na	SMB	na	4	na	m	−13 803.5 ± 2.8	212.8 ± [4.7]	1970COX/PIL,1951MAG/HAR

Recommendation

$\Delta_f H_m^o$ (cr, 298.15 K)	212.8 ± 4.7 kJ mol^{-1}	Available value	Entry 1

Evaluation

The value given by Magnus *et al.* [1951MAG/HAR] was analyzed and recalculated by Cox and Pilcher [1970COX/PIL].

7.57.2. Enthalpy of fusion

None available.

7.57.3. Enthalpy of vaporization

None available.

7.57.4. Enthalpy of sublimation

TABLE 279. Sublimation enthalpy of 9,9′-biphenanthrene

Entry	T_{Range} K	$\Delta_{\text{sub}}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H_m^o$(298.15 K) kJ mol^{-1}	Method	Purity %	Reference
1	na	151.5	na	na	na	na	1951MAG/BEC

Evaluation

There are no details available (see the value estimated).

7.57.5. Summary

TABLE 280. A summary of estimated phase change enthalpies for 9,9′-biphenanthrene

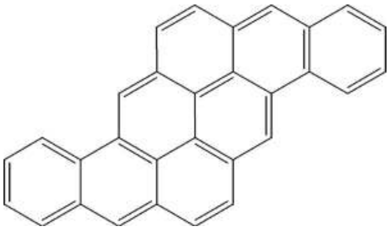
	$\Delta_{\text{fus}}H_m(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{fus}}H_m^o$(298 K) kJ mol^{-1}	$\Delta_{\text{vap}}H_m^o$(298 K) kJ mol^{-1}	$\Delta_{\text{sub}}H_m^o$(298 K) kJ mol^{-1}	$\Delta_{\text{fus}}H_m^o$(298 K) + $\Delta_{\text{vap}}H_m^o$(298 K) kJ mol^{-1}
expt.				151.5	
estimated	25.6		134.3		159.9

[a]Sum of the estimated fusion and vaporization enthalpies; T_{fus}=457 K; estimated $\Delta_{\text{tpce}}S(T_{\text{fus}})$=58.2 J mol^{-1} K^{-1}.

TABLE 281. A summary of estimated enthalpy of sublimation and formation in the gas phase of 9,9′-biphenanthrene

$\Delta_f H_m^o$(cr, 298.15 K) kJ mol^{-1}	$\Delta_{\text{sub}}H_m^o$(298.15 K) kJ mol^{-1}	$\Delta_f H_m^o$(g, 298.15 K) kJ mol^{-1}
212.8 ± 4.7	151.5	364

7.58. Pyranthrene



Name	Formula	Registry Number	Molecular Weight
Pyranthrene	$C_{30}H_{16}$	[191-13-9]	376.448 04 g mol^{-1}

7.58.1. Enthalpy of formation (solid)

None available.

7.58.2. Enthalpy of fusion

None available

7.58.3. Enthalpy of vaporization

None available.

7.58.4. Enthalpy of sublimation

TABLE 282. Sublimation enthalpy of pyranthrene

Entry	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	194.3 ± 10	595	213.0 ± 11.8	ME	na	1952INO/SHI

[a] sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid pyranthrene of 401.4 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}$ (298.15 K)	213.0 ± 11.8 kJ mol^{-1}	Available value	Entry 1

7.58.5. Summary

TABLE 283. A summary of experimental and estimated phase change enthalpies for pyranthrene

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.				213.0 ± 11.8	
estimated	na[a]		143.7		

[a] Melting point not available.

7.59. *p*-Quinquephenyl

Name	Formula	Registry Number	Molecular Weight
p-Quinquephenyl	$C_{30}H_{22}$	[3073-05-0]	382.495 68 g mol^{-1}

7.59.1. Enthalpy of formation (solid)

None available.

7.59.2. Enthalpy of fusion

TABLE 284. Fusion enthalpy of *p*-quinquephenyl

Entry	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	T_{fus} K	$\Delta_{\mathrm{trans}}H_{\mathrm{m}}(T_{\mathrm{trans}})$ kJ mol^{-1}	T_{trans} K	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	Method	Purity %	Reference
1	42.3 ± 5.4	659.6	0.9 ± 0.1[a]	688.1	7.7 ± 12.9[b]	DSC	na	1979SMI

[a] Liquid crystal (nematic to isotropic transition).

[b] Adjustment of the fusion enthalpy to $T=298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid *p*-quinquephenyl of 602 and 453 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{fus}H_m$ (T_{fus})	42.3 ± 5.4 kJ mol^{-1}	Available value	Entry 1
$\Delta_{fus}H^o_m$ (298.15 K)	7.7 ± 12.9 kJ mol^{-1}	Available value	Entry 1

Evaluation

The fusion enthalpy was adjusted to 298.15 K as noted above; the uncertainty in this value includes the standard deviation of the measurements ($\pm 2\sigma$) as well as an estimate of the uncertainty associated with the temperature adjustment.

7.59.3. Enthalpy of vaporization

None available.

7.59.4. Enthalpy of sublimation

None available.

7.59.5. Summary

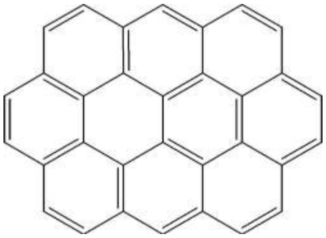
TABLE 285. A summary of experimental and estimated phase change enthalpies for *p*-quinquephenyl

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) + $\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}
expt.	42.3 ± 5.4	7.7 ± 12.9			
estimated	67.7[a]		143.7		211.4[b]

[a] Fusion enthalpies of liquid crystals are overestimated.

[b] The sum of the experimental fusion enthalpy and estimated vaporization enthalpy; estimated $\Delta_{tpce}S(T_{fus}) = 102.8$ J mol^{-1} K^{-1}.

7.60. Ovalene



Name	Formula	Registry Number	Molecular Weight
Ovalene	$C_{32}H_{14}$	[190-26-1]	398.453 56 g mol^{-1}

7.60.1. Enthalpy of formation (solid)

None available.

7.60.2. Enthalpy of fusion

TABLE 286. Fusion enthalpy of ovalene

Entry	$\Delta_{trans}H_m(T_{trans})$ kJ mol^{-1}	T_{trans} K	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	T_{fus} K	$\Delta_{tpce}H^o_m$(298 K) kJ mol^{-1}	Method	Purity %	Reference
1	8.1 ± 1.0	729	17.4 ± 2.2	770	na[a]	DSC	na	1980SMI

[a] Eq. (5) is not applicable over this temperature range; adjustment of the fusion enthalpy to $T = 298.15$ K using Eq. (5) and estimated heat capacities for liquid and solid ovalene result in a negative fusion enthalpy.

Recommendation

$\Delta_{\text{tpce}}H_{\text{m}}(T_{\text{fus}})$	25.5 ± 2.4 kJ mol^{-1}	Available value	Entry 1
$\Delta_{\text{tcpe}}H^{\text{o}}_{\text{m}}(298.15\ \text{K})$	not available		

7.60.3. Enthalpy of vaporization

None available.

7.60.4. Enthalpy of sublimation

TABLE 287. Sublimation enthalpy of ovalene

Entry	T_{Range} K	$\Delta_{\text{sub}}H_{\text{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\ \text{K})^{\text{a}}$ kJ mol^{-1}	Method	Purity %	Reference
1	550–650	211.3 ± 16	600	230 ± 17[a]	ME	na	1987STE/MAL, 1952INO/SHI

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid ovalene of 404 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298.15\ \text{K})$	230 ± 17 kJ mol^{-1}	Available value	Entry 1

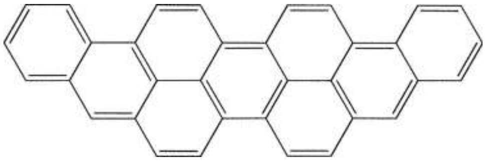
7.60.5. Summary

TABLE 288. A summary of experimental and estimated phase change enthalpies for ovalene

	$\Delta_{\text{tpce}}H_{\text{m}}(T_{\text{fus}})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\ \text{K})$ kJ mol^{-1}	$\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\ \text{K})$ kJ mol^{-1}	$\Delta_{\text{sub}}H^{\text{o}}_{\text{m}}(298\ \text{K})$ kJ mol^{-1}	$\Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298\ \text{K})+\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298\ \text{K})$ kJ mol^{-1}
expt.	25.5 ± 2.4			230 ± 17	
estimated	28.2		153.1		181.3[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\text{tpce}}S(T_{\text{fus}})=102.8$ J mol^{-1} K^{-1}.

7.61. Violanthrene A



Name	Formula	Registry Number	Molecular Weight
Violanthrene A, anthra[9,1,2-*cde*]benzo [*rst*] pentaphene	$C_{34}H_{18}$	[81-31-2]	426.506 72 g mol^{-1}

7.61.1. Enthalpy of formation (solid)

None available.

7.61.2. Enthalpy of fusion

None available; T_{fus}: 751 K.

7.61.3. Enthalpy of vaporization

None available.

7.61.4. Enthalpy of sublimation

TABLE 289. Sublimation enthalpy of violanthrene A

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H^o_m(298.15\ K)^a$ kJ mol^{-1}	Method	Purity %	Reference
1	560–630	196.4	600^a	218.9	ME	na	1967WAK/INO
2	590	223.6 ± 17.6	590	245.4 ± 19	ME	na	1952INO/SHI

[a] Temperature range approximate.

[b] Sublimation enthalpies adjusted to T=298.15 K using Eq. (3) and an estimated heat capacity for solid violanthrene of 453.4 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H^o_m(298.15\ K)$	232 ± 19 kJ mol^{-1}	Available value	Entries 1 and 2

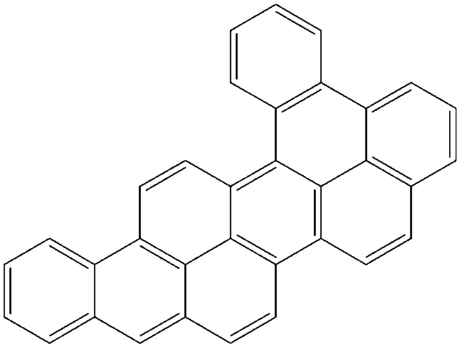
7.61.5. Summary

TABLE 290. A summary of experimental and estimated phase change enthalpies for violanthrene A

	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298\ K)$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298\ K)+\Delta_{vap}H^o_m(298\ K)$ kJ mol^{-1}
expt.				232 ± 19	
estimated	30.3		162.5		192.8^a

[a] The sum of the estimated fusion and vaporization enthalpy using the melting point of 751 K; $\Delta_{tpce}S(T_{fus})$=40.4 J mol^{-1} K^{-1}.

7.62. Violanthrene B



Name	Formula	Registry Number	Molecular Weight
Violanthrene B, dibenzo [*a*,*rst*] naphtho[8,1,2-*cde*]-pentaphene	$C_{34}H_{18}$	[81-31-2]	426.506 72 g mol^{-1}

7.62.1. Enthalpy of formation (solid)

None available.

7.62.2. Enthalpy of fusion

None available; T_{fus}: 603 K.

7.62.3. Enthalpy of vaporization

None available.

7.62.4. Enthalpy of sublimation

TABLE 291. Sublimation enthalpy of violanthrene B

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})^{\mathrm{a}}$ kJ mol^{-1}	Method	Purity %	Reference
1	475–625	154.1[a]	550	173[b]	ME	na	1967WAK/INO

[a] Temperature range approximate.
[b] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid violanthrene B of 453.4 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	173 kJ mol^{-1}	Available value	Entry 1

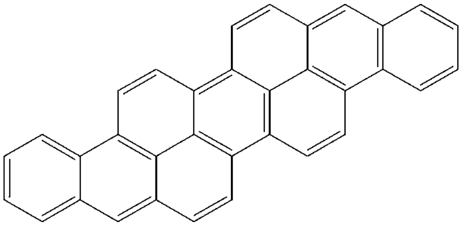
7.62.5. Summary

TABLE 292. A summary of experimental and estimated phase change enthalpies for violanthrene B

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}298\ \mathrm{K})$ kJ mol^{-1}
expt.				173	
estimated	24.4		162.5		186.9[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=40.4$ J mol^{-1} K^{-1}.

7.63. Isoviolanthrene A



Name	Formula	Registry Number	Molecular Weight
Isoviolanthrene A, benzo [*rst*] phenanthro[10,1,2-*cde*] pentaphene	$C_{34}H_{18}$	[188-87-0]	426.506 72 g mol^{-1}

7.63.1. Enthalpy of formation (solid)

None available.

7.63.2. Enthalpy of fusion

None available; T_{fus}: 783 K.

7.63.3. Enthalpy of vaporization

None available.

7.63.4. Enthalpy of sublimation

Table 293. Sublimation enthalpy of isoviolanthrene A

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})^{\mathrm{a}}$ kJ mol^{-1}	Method	Purity %	Reference
1	570–725	219	650$^{\mathrm{a}}$	245$^{\mathrm{b}}$	ME	na	1967WAK/INO

[a] Temperature range approximate.

[b] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat capacity for solid isoviolanthrene A of 453.4 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})$	245 kJ mol^{-1}	Available value	Entry 1

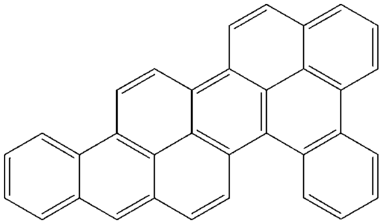
7.63.5. Summary

Table 294. A summary of experimental and estimated phase change enthalpies for isoviolanthrene A

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}^{\mathrm{o}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.				245	
estimated	31.6		162.5		194.1$^{\mathrm{a}}$

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=40.4$ J mol^{-1} K^{-1}.

7.64. Isoviolanthrene B



Name	Formula	Registry Number	Molecular Weight
Isoviolanthrene B, phenanthro[1,10,9,8-*opqra*] perylene	$C_{34}H_{18}$	[190-93-2]	426.506 72 g mol^{-1}

7.64.1. Enthalpy of formation (solid)

None available.

7.64.2. Enthalpy of fusion

None available; T_{fus}: 603.2 K [1987STE/MAL].

7.64.3. Enthalpy of vaporization

None available

7.64.4. Enthalpy of sublimation

Table 295. Sublimation enthalpy of isoviolanthrene B

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}^{\mathrm{o}}(298.15\ \mathrm{K})^{\mathrm{a}}$ kJ mol^{-1}	Method	Purity %	Reference
1	478–603	154.1	540.5	171$^{\mathrm{a}}$	na	na	1987STE/MAL

[a]Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat for solid isoviolanthrene B of 543.4 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H_m^o(298.15\text{ K})$	171 kJ mol^{-1}	Questionable value	Entry 1

7.64.5. Summary

TABLE 296. A summary of experimental and estimated phase change enthalpies for isoviolanthrene B

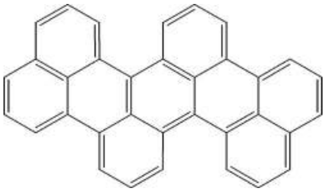
	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\text{ K})$ kJ mol^{-1}	$\Delta_{vap}H_m^o(298\text{ K})$ kJ mol^{-1}	$\Delta_{sub}H_m^o(298\text{ K})^a$ kJ mol^{-1}	$\Delta_{fus}H_m^o(298\text{ K})+\Delta_{vap}H_m^o(298\text{ K})$ kJ mol^{-1}
expt.				171	
estimated	24.4		162.5		186.9^a

[a]Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})=40.4$ J mol^{-1} K^{-1}.

Evaluation

The sublimation enthalpy is questionable.

7.65. Tetrabenzo[*de*,*hi*,*op*,*st*]pentacene



Name	Formula	Registry Number	Molecular Weight
Tetrabenzo[*de*,*hi*,*op*,*st*]pentacene	$C_{34}H_{18}$	[191-79-7]	426.506 72 g mol^{-1}

7.65.1. Enthalpy of formation (solid)

None available.

7.65.2. Enthalpy of fusion

None available; T_{fus}: 606 K [1987STE/MAL].

7.65.3. Enthalpy of vaporization

None available.

7.65.4. Enthalpy of sublimation

TABLE 297. Sublimation enthalpy of tetrabenzo[*de*,*hi*,*op*,*st*]pentacene

Entry	T_{Range} K	$\Delta_{sub}H_m(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{sub}H_m^o(298.15\text{ K})^a$ kJ mol^{-1}	Method	Purity %	Reference
1	348–448	118.5	398	127.1^a	na	na	1987STE/MAL 1967WAK/INO

[a]Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat for solid tetrabenzo[*de*,*hi*,*op*,*st*]pentacene of 453 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{sub}H_m^o$ (298.15 K)	127.1 kJ mol^{-1}	Highly questionable value	Entry 1

7.65.5. Summary

TABLE 298. A summary of experimental and estimated phase change enthalpies for tetrabenzo[*de*,*hi*,*op*,*st*]pentacene

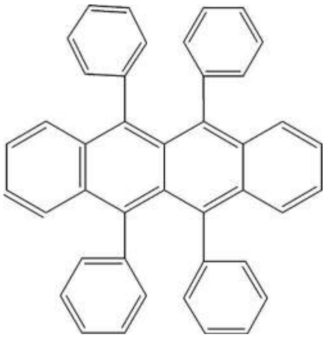
	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{vap}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{sub}H^o_m$(298 K) kJ mol^{-1}	$\Delta_{fus}H^o_m$(298 K)+ $\Delta_{vap}H^o_m$(298 K) kJ mol−1
expt.				127.1	
estimated	24.5		162.5		187.0[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{tpce}S(T_{fus})$=40.4 J mol^{-1} K^{-1}.

Evaluation

The experimental sublimation enthalpy is highly questionable.

7.66. 5,6,11,12-Tetraphenyltetracene



Name	Formula	Registry Number	Molecular Weight
5,6,11,12-Tetraphenyltetracene, rubrene	$C_{42}H_{28}$	[517-51-1]	532.67 72 g mol^{-1}

7.66.1. Enthalpy of formation (solid)

TABLE 299. Standard enthalpies of combustion and formation of 5,6,11,12-tetraphenyltetracene at T=298.15 K

Entry	Purity %	Method	Charact.	Num. of exp.	Aux. Subs.	Amount Reactn.	$\Delta_rH^o_m$(cr) kJ mol^{-1}	$\Delta_fH^o_m$(cr) kJ mol^{-1}	Reference
1	na	SMB	na	4	na	m	−21149.3±21.3	620±22	1970COX/PIL, 1938END

Recommendation

$\Delta_fH^o_m$ (cr,298.15 K)	620±22 kJ mol^{-1}	Questionable value	Entry 1

Evaluation

The experimental combustion and formation enthalpy is questionable.

7.66.2. Enthalpy of fusion

None available; T_{fus}: 604.2 K [1987STE/MAL].

7.66.3. Enthalpy of vaporization

None available.

7.66.4. Enthalpy of sublimation

TABLE 300. Sublimation enthalpy of 5,6,11,12-tetraphenyltetracene

Entry	T_{Range} K	$\Delta_{\mathrm{sub}}H_{\mathrm{m}}(\bar{T})$ kJ mol^{-1}	$\bar{T}$ K	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})^{\mathrm{a}}$ kJ mol^{-1}	Method	Purity %	Reference
1	453–523	160.8	488	180.6	na	na	1987STE/MAL, 1958HOY/PEP

[a] Sublimation enthalpies adjusted to $T=298.15$ K using Eq. (3) and an estimated heat for solid 5,6,11,12-tetraphenyltetracene of 609 J mol^{-1} K^{-1}.

Recommendation

$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}$ (298.15 K)	180.6 kJ mol^{-1}	Questionable value	Entry 1

7.66.5. Summary

TABLE 301. A summary of experimental and estimated phase change enthalpies for 5,6,11,12-tetraphenyltetracene

	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})+\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298\ \mathrm{K})$ kJ mol^{-1}
expt.				180.6	
estimated	61.7		200.0		261.7[a]

[a] Sum of the estimated fusion and vaporization enthalpies; estimated $\Delta_{\mathrm{tpce}}S(T_{\mathrm{fus}})=102.2$ J mol^{-1} K^{-1}.

Evaluation

The experimental sublimation enthalpy is questionable.

TABLE 302. A summary of available enthalpy of sublimation and formation in the gas phase of 5,6,11,12-tetraphenyltetracene

$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}(\mathrm{cr},298.15\ \mathrm{K})$ / kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298.15\ \mathrm{K})$ / kJ mol^{-1}	$\Delta_{\mathrm{f}}H^{\mathrm{o}}_{\mathrm{m}}(\mathrm{g},298.15\ \mathrm{K})$ / kJ mol^{-1}
620 ± 22	262 (estimated)	882 (estimated)

8. Summary

The thermochemical values for the PAHs are summarized in the following table. Recommended values are in bold, suggested values are underlined, and values that are suspect are in italics. Values in italics were chosen as those outliers in Fig. 2. Single values and data difficult to recommend without other evidence are reported in normal font. In some cases where additional enthalpic transitions occur below the melting point but above 298.15 K, the sum is included under the $\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ column as indicated.

TABLE 303. Summary of the phase change enthalpies of the PAHs.

Formula	Compound	Experimental				Estimated		
		$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298)$ kJ mol^{-1}	$\Delta_{\mathrm{sub}}H^{\mathrm{o}}_{\mathrm{m}}(298)$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H^{\mathrm{o}}_{\mathrm{m}}(298) + \Delta_{\mathrm{vap}}H^{\mathrm{o}}_{\mathrm{m}}(298)$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})$ kJ mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{m}}(298)$ kJ mol^{-1}	$\Delta_{\mathrm{fus}}H_{\mathrm{m}}(T_{\mathrm{fus}})+\Delta_{\mathrm{vap}}H_{\mathrm{m}}(298)$ kJ mol^{-1}
C_6H_6	benzene	**9.90 ± 0.05**	**33.92 ± 0.06**	**44.7 ± 0.2**	**44.4 ± 0.2**	12.0	31.1	43.1
C_7H_8	toluene	**6.64 ± 0.01**	**38.06 ± 0.04**		**48.0 ± 1.1**	8.0	35.8	43.8
C_9H_8	indene	**10.20 ± 0.01**	50.6 ± 1.5		61.8 ± 1.5	11.6	45.2	56.8
C_9H_{10}	indane	**8.6 ± 0.1**	**49.2 ± 1.0**		**60.6 ± 1.4**	10.2	45.2	55.4
$C_{10}H_8$	naphthalene	**19.06 ± 0.08**	**55.4 ± 1.4**	**72.6 ± 0.3**	**72.3 ± 1.6**	15.6	49.9	65.5
$C_{12}H_8$	biphenylene	22.6 ± 0.7	66.4 ± 1.7	83.8 ± 0.6	85.1 ± 2.2	18.2	59.3	77.5
$C_{12}H_8$	acenaphthylene	6.94	66.9 ± 4.5	**72.5 ± 1.2**	70.9 ± 4.6	13.6	59.3	72.9
$C_{12}H_{10}$	acenaphthene	**21.46 ± 0.02**	**66.5 ± 0.2**	**84.8 ± 0.4**	**84.9 ± 1.1**	15	59.3	74.3
$C_{12}H_{10}$	biphenyl	**18.57 ± 0.01**	**64.9 ± 1.3**	**82.1 ± 2.1**	**81.5 ± 1.5**	20.2	59.3	79.5
$C_{13}H_{10}$	fluorene	**19.58 ± 0.06**	72.1 ± 1.9	86.5 ± 1.3	87.4 ± 2.4	19.7	64.0	83.7
$C_{13}H_{12}$	diphenylmethane	**19.01 ± 0.01**	**67.9 ± 0.4**	**87.2 ± 0.7**	**86.9 ± 0.4**	18.5	59.3	77.8
$C_{14}H_8$	pyracylene			83.2			68.7	
$C_{14}H_{10}$	anthracene	**29.4 ± 0.1**	79.9 ± 4.0	**101.9 ± 1.3**	99.6 ± 5.1	21.5	68.7	90.2
$C_{14}H_{10}$	phenanthrene	**16.46 ± 0.04**	**78.3 ± 1.8**	**92.1 ± 0.6**	**91.2 ± 2.2**	16.4	68.7	85.1
$C_{14}H_{12}$	pyracene			89.6 ± 3.3		18.3	68.7	87.0
$C_{16}H_{10}$	pyrene	**17.36 ± 0.04**	89.4 ± 3.1	**100.3 ± 1.0**	99.6 ± 3.9	18.1	78.0	96.1
$C_{16}H_{10}$	fluoranthene	**18.73 ± 0.02**	87.1 ± 3.6	101.2 ± 2.8	101.0 ± 3.9	17.6	78.0	95.6
$C_{16}H_{14}$	1-phenylnaphthalene		*88.6*			18.7	78.0	
$C_{17}H_{12}$	11*H*-benzo[*a*]fluorene	22.2 ± 0.8[a]	*83.7*	*105.4*	*96.1*	23.4	82.7	106.1
$C_{17}H_{12}$	11*H*-benzo[*b*]fluorene	23.4 ± 0.6	97.5 ± 5.8	122.0 ± 2.8	109.5 ± 6.9	24.8	82.7	107.5
$C_{18}H_{12}$	naphthacene	36.9[a]		135.9 ± 5.1		25.5	87.4	112.9
$C_{18}H_{12}$	benz[*a*]anthracene	21.4 ± 0.3	105.8 ± 3.8	119.5 ± 5.0	118.7 ± 4.7	19.0	87.4	106.4
$C_{18}H_{12}$	triphenylene	**24.74 ± 0.01**	106.1 ± 7.8	120.1 ± 3.3	120.0 ± 8.6	20.6	87.4	108.0
$C_{18}H_{12}$	chrysene	26.2 ± 0.2	106.2 ± 8.6	123.4 ± 4.2	121.0 ± 9.8	23.3	87.4	110.7
$C_{18}H_{12}$	benzo[*c*]phenanthrene	16.3 ± 1.4		*106.3*		14.7	87.4	102.1
$C_{18}H_{14}$	*p*-terphenyl	**35.4 ± 0.1**	101.2 ± 6.9	125.6 ± 1.6	124.7 ± 7.9	35.8	87.4	123.2
$C_{18}H_{14}$	*o*-terphenyl	**17.19 ± 0.1**	86.4 ± 4.4	103.0 ± 0.8	101.6 ± 4.5	24.2	87.4	111.6
$C_{18}H_{14}$	*m*-terphenyl	31.0 ± 0.4	*98.8*	**118.4 ± 2.4**	*125.8*	26.6	87.4	114.0
$C_{18}H_{14}$	5,12-dihydrotetracene			118.9 ± 1.0		26.1	87.4	113.5
$C_{19}H_{16}$	triphenylmethane	20.7 ± 0.4	93.8 ± 2.1	108.4 ± 2.8	109.8 ± 2.6	26.1	87.4	113.5
$C_{20}H_{12}$	corannulene	17.3 ± 1.2	112.4 ± 1.9	116.3 ± 7.0[b]	113.2 ± 5.9	17.9	96.8	114.7
$C_{20}H_{12}$	perylene	**31.87 ± 0.08**	118.5 ± 1.2	135.9 ± 2.6	133.1 ± 5.8	31.6	96.8	128.7
$C_{20}H_{12}$	benzo[*a*]pyrene	17.3 ± 0.6	116.7 ± 2.3	120.5 ± 2.7	123.4 ± 4.2	19.2	96.8	116.0
$C_{20}H_{12}$	benzo[*e*]pyrene	16.6 ± 0.8	118.2 ± 0.6	123.0 ± 1.8	126.6 ± 4.3	19.2	96.8	116
$C_{20}H_{12}$	benzo[*k*]fluoranthene	27.5 ± 0.1	117.4 ± 2.2	133.8 ± 4.5	131.9 ± 4.8	17.4	96.8	113.2
$C_{20}H_{12}$	2:3-benzofluoranthene		116.8 ± 3.2	*119.2*		15.6	96.8	112.4
$C_{20}H_{14}$	9-phenylanthracene	25.5 ± 0.8	103.8 ± 3.5	120.5 ± 3.4	120.2 ± 4.6	25.1	96.8	121.9

TABLE 303. Summary of the phase change enthalpies of the PAHs.—Continued

		Experimental				Estimated		
Formula	Compound	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{vap}H^o_m(298)$ kJ mol^{-1}	$\Delta_{sub}H^o_m(298)$ kJ mol^{-1}	$\Delta_{fus}H^o_m(298)$ + $\Delta_{vap}H^o_m(298)$ kJ mol^{-1}	$\Delta_{fus}H_m(T_{fus})$ kJ mol^{-1}	$\Delta_{vap}H_m(298)$ kJ mol^{-1}	$\Delta_{fus}H_m(T_{fus})+$ $\Delta_{vap}H_m(298)$ kJ mol^{-1}
$C_{22}H_{12}$	benzo[*ghi*]perylene	17.5 ± 0.2	128.9 ± 3.0	132.9 ± 2.3	128.9 ± 7.0	22.7	106.2	128.9
$C_{22}H_{14}$	1,2:3,4-dibenzanthracene	25.8 ± 0.1	132.3 ± 3.6	145.9 ± 6.0	139.2 ± 7.2	24.1	106.2	130.3
$C_{22}H_{14}$	1,2:5,6-dibenzanthracene	31.2 ± 1.0	131.1 ± 2.8	148.9 ± 4.2	144.1 ± 6.7	23.7	106.2	129.9
$C_{22}H_{14}$	pentacene			165.5 ± 12.3			106.2	
$C_{22}H_{14}$	picene	35.2 ± 0.8		149.4 ± 2.9		27.8	106.2	134.0
$C_{22}H_{14}$	1,2:6,7-dibenzophenanthrene			144.4 ± 2.5		24.6	106.2	130.8
$C_{24}H_{12}$	coronene	19.6 ± 2.4[a]	139.5 ± 6.0	142.6 ± 8.7		28.1	115.6	143.7
$C_{24}H_{14}$	1,2:4,5-dibenzopyrene	30.5 ± 1.1		155.2		22.0	115.6	137.6
$C_{24}H_{14}$	dibenzo[*b*,*def*]chrysene			144.3		22.7	115.6	138.3
$C_{24}H_{14}$	benzo[*r*,*s*,*t*]pentaphene	27.9 ± 1.2				23.5	115.6	139.1
$C_{24}H_{14}$	dibenzo[*fg*,*op*]chrysene			157.2		25.9	115.6	141.5
$C_{24}H_{18}$	1,3,5-triphenylbenzene	32.4 ± 1.3	133.4 ± 4.0	**149.8** ± **1.6**	153.8 ± 5.7	39.4	115.6	155.0
$C_{24}H_{18}$	p-quaterphenyl	57.6 ± 0.9	136.1 ± 3.2		172.5 ± 8.4	51.8	115.6	167.4
$C_{25}H_{20}$	tetraphenylmethane	48.3 ± 0.2		140.0 ± 2.6		41.5	116.9	158.4
$C_{26}H_{16}$	tetrabenzonaphthalene			150.9		21.2	124.9	146.1
$C_{26}H_{18}$	9,10-diphenylanthracene		*102.7*	169.6 ± 5.9		38.2	124.9	163.1
$C_{26}H_{18}$	9,9′-bifluorenyl	36.9		132.6 ± 2.3		37.4	124.9	162.3
$C_{28}H_{14}$	*meso*-naphthodianthrene			197.6 ± 11.5			134.3	
$C_{28}H_{18}$	9,9′-bianthracene			*148*			134.3	
$C_{28}H_{18}$	9,9′-bi-phenanthrene			*151.5*		25.6	134.3	159.9
$C_{30}H_{16}$	pyranthrene			213.0 ± 11.8			143.7	
$C_{30}H_{22}$	*p*-quinquephenyl	42.3 ± 5.4				67.7	143.7	211.4
$C_{32}H_{14}$	ovalene	25.5 ± 2.4[a]		230 ± 17		28.2	153.1	181.3
$C_{34}H_{18}$	violanthrene A			232 ± 19		30.3	162.5	192.8
$C_{34}H_{18}$	violanthrene B			173		24.4	162.5	186.9
$C_{34}H_{18}$	isoviolanthrene A			245		31.6	162.5	194.1
$C_{34}H_{18}$	isoviolanthrene B			*171*		24.4	162.5	186.9
$C_{34}H_{18}$	tetrabenzo[*de*,*hi*,*op*,*st*]pentacene			*127.1*		24.5	162.5	187.0
$C_{42}H_{28}$	5,6,11,12-tetraphenyltetracene			*180.6*		61.7	200.0	261.7

[a] Total phase change enthalpy.

[b] The average of the direct and indirect measurement.

Figure 1 illustrates the correlation between sublimation enthalpies measured directly and those obtained by summing the vaporization enthalpies with fusion enthalpies at $T=298.15$ K according to Eq. (4). The correlation between experimental sublimation enthalpies and those calculated from experimental data excluding suspected data according to Eq. (4) is given by

$$\Delta_{sub}H^o_m(298.15\ \text{K})/\text{kJ mol}^{-1} = (0.991 \pm 0.026)[\Delta_{vap}H^o_m(298.15\ \text{K}) + \Delta_{fus}H^o_m(298.15\ \text{K})] + (1.53 \pm 3.42) \quad (r^2 = 0.9812). \tag{11}$$

Similarly, the correlation between experimental sublimation enthalpies and those calculated from estimated values is illustrated in Fig. 2. Most of the scatter in Fig. 2 occurs with experimental sublimation enthalpies in excess of 160 kJ mol^{-1}, many compounds for which there are no experimental enthalpy values for fusion and vaporization in Fig. 1. The reasonable correlation observed for most compounds with experimental sublimation enthalpies less than 160 kJ mol^{-1}, Eq. (12), suggests that values in excess of this amount should be viewed with some skepticism. Equation (12) was generated by comparing experimental and estimated sublimation enthalpies up to 160 kJ:

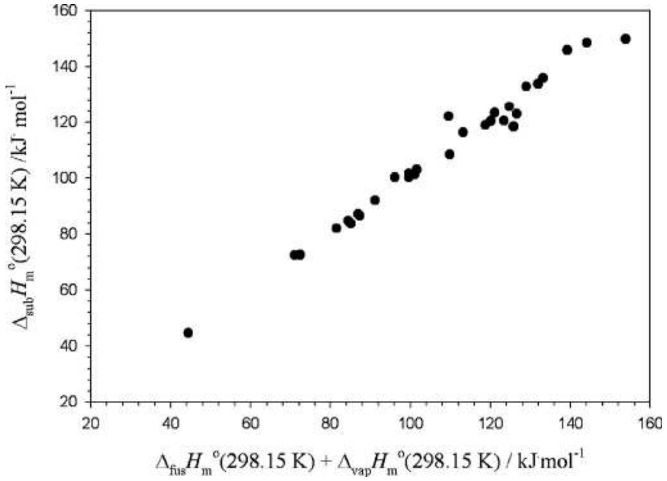


FIG. 1. A comparison of experimental sublimation enthalpies measured directly with those obtained from experimental vaporization and fusion enthalpies.

$$\Delta_{\text{sub}}H_{\text{m}}(298.15\ \text{K})/\text{kJ mol}^{-1} = (0.986 \pm 0.49)[\Delta_{\text{vap}}H^{\text{o}}_{\text{m}}(298.15\ \text{K}) + \Delta_{\text{fus}}H^{\text{o}}_{\text{m}}(298.15\ \text{K})]_{\text{estm}} + (8.18 \pm 8.1) \quad (r^2 = 0.9075). \tag{12}$$

The enthalpies of formation of the PAHs in both the condensed and vapor phases at $T=298.15$ K are summarized in the following table. Recommended values are in bold, suggested values are underlined, and values that are suspect are in italics.

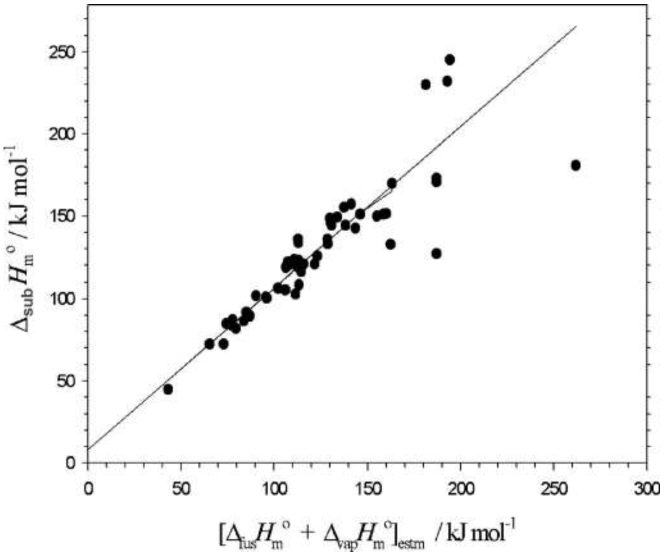


FIG. 2. A comparison of experimental sublimation enthalpies with those estimated. The line represents a comparison of experimental and estimated values up to 160 kJ mol^{-1}.

TABLE 304. A Summary of the enthalpies of sublimation and formation of PAHs.

Formula	Compound	$\Delta_f H^o_m$(cd, 298.15 K) kJ mol^{-1}	$\Delta_{sub/vap} H^o_m$(298.15 K) kJ mol^{-1}	$\Delta_f H^o_m$(g, 298.15 K) kJ mol^{-1}
C_6H_6	benzene (l)	**49.0 ± 0.9**	**33.9 ± 0.1**	**82.9 ± 0.9**
C_7H_8	toluene (l)	**12.0 ± 1.1**	**38.1 ± 0.1**	**50.1 ± 1.1**
C_9H_8	indene (l)	110.6 ± 1.8	50.6 ± 1.5	161.2 ± 2.3
C_9H_{10}	indane (l)	**11.7 ± 1.8**	**49.2 ± 1.0**	**60.9 ± 2.1**
$C_{10}H_8$	naphthalene	**78.0 ± 1.5**	**72.6 ± 0.3**	**150.6 ± 1.5**
$C_{12}H_8$	biphenylene	333.4 ± 1.8	83.8 ± 0.6	417.2 ± 1.9
$C_{12}H_8$	acenaphthylene	190.8 ± 3.5	**72.5 ± 1.2**	263.2 ± 3.7
$C_{12}H_{10}$	acenaphthene	72.0 ± 3.1	**84.8 ± 0.4**	156.8 ± 3.1
$C_{12}H_{10}$	biphenyl	**98.2 ± 2.5**	**82.1 ± 2.1**	**180.3 ± 3.3**
$C_{13}H_{10}$	fluorene	90.2 ± 2.8	86.5 ± 1.3	176.7 ± 3.1
$C_{13}H_{12}$	diphenylmethane (l)	97.1 ± 2.2	**67.9 ± 0.4**	165.0 ± 2.2
$C_{13}H_{12}$	diphenylmethane (c)	75.1 ± 2.2	**87.2 ± 0.7**	162.3 ± 2.3
$C_{14}H_8$	pyracylene	325.4 ± 3.6	83.2	408.6
$C_{14}H_{10}$	anthracene	**127.5 ± 2.6**	**101.9 ± 1.3**	**229.4 ± 2.9**
$C_{14}H_{10}$	phenanthrene	**110.1 ± 2.2**	**92.1 ± 0.6**	**202.2 ± 2.3**
$C_{14}H_{12}$	pyracene	84.7 ± 4.1	89.6 ± 3.3	174.3 ± 5.3
$C_{16}H_{10}$	pyrene	125.2 ± 2.3	**100.3 ± 1.0**	225.5 ± 2.5
$C_{16}H_{10}$	fluoranthene	190.2 ± 2.8	101.2 ± 2.8	291.4 ± 4.0
$C_{18}H_{12}$	naphthacene	206.7 ± 3.0	135.9 ± 5.1	342.6 ± 5.9
$C_{18}H_{12}$	benz[*a*]anthracene	170.8 ± 3.3	119.5 ± 5.0	290.3 ± 6.0
$C_{18}H_{12}$	triphenylene	150.0 ± 2.9	120.1 ± 3.3	270.1 ± 4.4
$C_{18}H_{12}$	chrysene	145.3 ± 2.2	123.4 ± 4.2	268.7 ± 4.7
$C_{18}H_{12}$	benzo[*c*]phenanthrene	184.9 ± 3.0	*106.3*	*291.2*
$C_{18}H_{14}$	*p*-terphenyl	158.8 ± 3.4	125.6 ± 1.6	284.4 ± 3.8
$C_{18}H_{14}$	*o*-terphenyl	179.8 ± 3.1	103.0 ± 0.8	282.8 ± 3.2
$C_{18}H_{14}$	*m*-terphenyl	**161.6 ± 3.1**	**118.4 ± 2.4**	**280.0 ± 3.9**
$C_{18}H_{14}$	5,12-dihydrotetracene	106.0 ± 2.7	118.9	
$C_{19}H_{16}$	triphenylmethane	167.7 ± 4.1	108.4 ± 2.8	276.1 ± 5.0
$C_{20}H_{12}$	corannulene	342.2 ± 6.0	116.3 ± 7.0	458.5 ± 9.2
$C_{20}H_{12}$	perylene	182.4 ± 2.7	135.9 ± 2.6	318.3 ± 3.7
$C_{20}H_{12}$	benzo[*k*]fluoranthene	172.4 ± 4.3	133.8 ± 4.5	306.2 ± 6.2
$C_{22}H_{14}$	1,2:3,4-dibenzanthracene	184.8 ± 8.7	145.9 ± 6.0	330.7 ± 10.6
$C_{22}H_{14}$	dibenz[*a*,*h*]anthracene	178.8 ± 10.2	148.9 ± 4.2	328 ± 11
$C_{24}H_{12}$	coronene	152.3 ± 6.9	142.6 ± 8.7	294.9 ± 11.1
$C_{24}H_{18}$	1,3,5-triphenylbenzene	222.0 ± 3.4	**149.8 ± 1.6**	371.8 ± 3.8
$C_{24}H_{18}$	*p*-quaterphenyl	227 ± 7	172.5 ± 8.4	400 ± 11
$C_{25}H_{20}$	tetraphenylmethane	247.2 ± 4.1	140 ± 2.6	387.2 ± 4.9
$C_{26}H_{16}$	tetrabenzonaphthalene	379 ± 37	150.9	530
$C_{26}H_{18}$	9,10-diphenylanthracene	308.7 ± 4.5	169.6 ± 5.9	478.3 ± 7.4
$C_{26}H_{18}$	9,9′-bifluoranyl	197.5 ± 3.5	132.6 ± 2.3	330.1 ± 4.2
$C_{28}H_{18}$	9,9′-bianthracene	326.9 ± 4.8	*148*	*475*
$C_{28}H_{18}$	9,9′-biphenanthrene	212.8 ± 4.7	*151.5*	364
$C_{42}H_{28}$	5,6,11,12-tetraphenyltetracene	620 ± 22	*262(est)*	*882 (est)*

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10. Appendix

TABLE 305. Acronyms used in the tables

a	aneroid
AC	adiabatic calorimetry
AM	absolute manometer
BAG	Baratron gauge
BG	Bourdon gauge
bp	boiling point
C	calorimetric determination
CE	comparative ebelliometry
cfm	calorimetric fractional melting
CG	calorimetric grade (Carlo Erba)
CGC	correlation-gas chromatography
CGC-DSC	combined correlation-gas chromatography differential scanning calorimetry
cryst	successive crystallization
DM	diaphram manometer
DC	drop calorimeter
DSC	differential scanning calorimeter
ea	elemental analysis
EM	electronic manometer
f	flame
fd	fractional distillation
fpd	freezing point depression
GC	gas chromatography
glc	gas-liquid chromathography
GS	gas saturation transpiration
H	hydrogenation reaction
HSA	head space analysis
I	isoteniscope
i	isoperibolic
IP	inclined piston
KG	Knudsen gauge
LC	liquid chromathography
LE	Langmuir evaporation
ME	mass effusion–Knudsen effusion
MG	McLeod gauge
MM	mercury manometer
mp	melting point
na	not available
OAS	organic analytical standard grade
P-BP	boiling point measured as a function of pressure
P/CO_2	determination from the mass of carbon dioxide formed by combustion
PG	pressure gauge
QF	quartz fiber
QC	quartz crystal
QHG	quartz helix gauge
RC	radiation calorimeter
RG	Rodebush gauge
RMB	rotating macrobomb
rmb	rotating microbomb
SRFG	spinning rotor friction gauge
SMB	static macrobomb
smb	static micro bomb
Sub	sublimation under vacuum
TE	torsion effusion
Tfmp	thin-film melting points apparatus
TSGC	temperature scanning gas chromatography
VFC	vapor flow calorimetry
VG	viscosity gauge
VLRS	vapor liquid recirculating still
Zrm	zone refining melting

TABLE 306. Groups used for liquid [$\Gamma(1)$] and solid [$\Gamma(c)$] heat capacity estimations from [1993CHI/HES]

	$\Gamma(1)$	$\Gamma(c)$
Hydrocarbon Group	$J\ mol^{-1}\ K^{-1}$	$J\ mol^{-1}\ K^{-1}$
primary sp^3 carbon	34.9	36.6
secondary sp^3 carbon	31.9	26.9
tertiary sp^3 carbon	22.4	9
quaternary sp^3 carbon	14	−5
secondary sp^2 carbon	25.8	46
tertiary sp^2 carbon	27.8	21.4
quaternary sp^2 carbon	21.7	6.9
tertiary sp carbon	34.3	37.1
quaternary sp carbon	28.9	15.5
tertiary aromatic sp^2 carbon	21.8	17.5
quaternary aromatic sp^2	15.3	8.5
internal quaternary aromatic carbon	16	9.1
cyclic secondary sp^3 carbon	25.9	24.6
cyclic tertiary sp^3 carbon	20.6	11.7
cyclic quaternary sp^3 carbon	18	6.1
cyclic tertiary sp^2	21.8	15.9
cyclic quaternary sp^2	21.2	4.7

TABLE 307. Groups values used for estimating total phase change entropies for PAHs

Aliphatic and Aromatic Carbon Groups	Group Notation	Group Value(G_i) J mol^{-1} k^{-1}
pimary sp^3 carbon atom	CH$_3$—R	17.6
secondary sp^3 carbon atom	R—CH$_2$—R	7.1
quaternary sp^3	CR$_4$	−10.7
tertiary aromatic sp^2	═CH—	7.4
quaternary aromatic sp^2 adjacent to an sp^3 atom	═C(R1)—	−9.6
peripheral quaternary aromatic sp^2 carbon adjacent to an sp^2 atom	═C(R2)—	−7.5
internal quaternary sp^2 adjacent to an sp^2 atom	═C(R3)—	−0.7

TABLE 308. Contributions of the cyclic hydrocarbon portions of the molecule from [2003CHI/ACR2].

Contributions of cyclic carbons on five-membered rings	Group Notation	Group Value(G_i) J mol^{-1} K^{-1}
cyclic tertiary sp^3 carbon	—CH(R)—	−14.7
cyclic quaternary sp^3 carbon	—C(R)$_2$—	−34.6
cyclic tertiary sp^2 carbon	═CH—	−1.6
cyclic quaternary sp^2 carbon	═C(R)—	−12.3

The ring equation for nonaromatic cyclic compounds containing a five-membered saturated or unsaturated ring (see 2003CHI/ACR2for more details) is $\Delta S_{\mathrm{ring}}=33.4N+3.7(R-3N)$, where R is the total number of ring atoms in the five-membered ring and N is the number of the five-membered ring

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