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Recommended Vapor Pressure of Solid Naphthalene

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Recommended vapor pressures of solid naphthalene, which are consistent with calorimetric enthalpies of sublimation and also with properties at the triple point temperature (vapor pressure, enthalpy of vaporization and enthalpy of fusion), were established. The recommended data were developed by a multiproperty simultaneous correlation of vapor pressures and related thermal data. Vapor pressures measured in this work by a static method in the temperature range from (273 to 313) K, covering pressure range from (0.8 to 45) Pa, were included in the simultaneous correlation. Effect of thermal transpiration was found to be negligible in this pressure range.

Introduction

Naphthalene was suggested as a reference compound for vapor pressure measurements below $p = 1000$ Pa[1−4] as well as for enthalpy of sublimation and heat capacity measurements.[5,6] While data for the liquid phase seem to be well-established,[7,8] results in the solid phase are scattered, and data reconciliation is desirable.

The aim of the present work was to develop recommended sublimation vapor pressure of naphthalene, consistent with calorimetric enthalpies of sublimation and also with properties at the triple point temperature, which are well-established. Vapor pressures in the solid phase were measured by a static method in the temperature range from (273 to 313) K, covering pressure range from 0.8 Pa to 45 Pa. Measurements at lower temperatures (down to 248 K) were performed in order to explore the capability of our apparatus; these values can be, however, subject of systematic errors and were not included in the correlation. Data were treated simultaneously with the selected literature data on enthalpies of sublimation and on differences of heat capacities of perfect gas and that of solid. Resulting parameters of the Cox equation were constrained to agree with the recommended vapor pressure and enthalpy of vaporization at the triple point.

As suggested by de Kruif et al.,[9] we used naphthalene as the first compound to be measured in our new apparatus with the objective to contribute to the establishment of recommended sublimation pressures and enthalpies of sublimation for this compound.

Experimental Section

Sample. Commercially available naphthalene (Aldrich 99+ %) was purified by zone refining. Analysis by gas chromatography (Hewlett-Packard 6890 gas chromatograph equipped with column HP5 cross-linked 5 % PH ME siloxane, length 30 m, film thickness 0.25 μm, i.d. 0.32 mm, and FID detector) showed no detectable impurities.

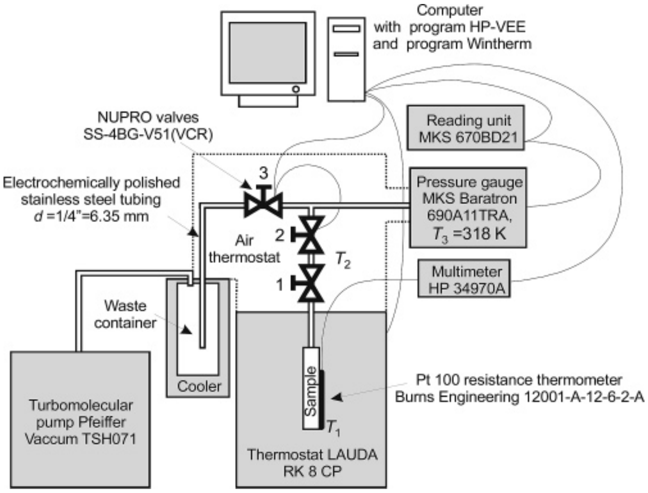

Figure 1. Static apparatus for the measurement of vapor pressure. Valves 2 and 3 are computer controlled and take control of measuring procedure. Valve 1 is the container valve. $T_1 < T_2 < T_3$.

Perfect degassing of the sample is a prerequisite for correct vapor pressure measurement by a static method. We used a method of pumping out gases above the sample placed in a measuring cell. A semipermeable membrane made of poly(dimethylsiloxane), which is permeable only for low molecular weight gases (oxygen, nitrogen, etc.) but not for the sample molecules, was placed between the sample cell and the vacuum pump to avoid loss of the material when the vapor space was pumped out. The pressure was maintained at or below 1 Pa to efficiently remove low molecular weight gases. At least 2 weeks was allowed to ensure complete degassing. No sample agitation was made during the degassing.

Apparatus. Vapor pressure was measured by a static method using an apparatus shown in Figure 1. It was constructed of 1/4 in. stainless steel internally electrochemically polished tubing with VCR fittings and Nupro valves (Swagelok Co., USA). Tubing was heated to 315 K to prevent condensation of the sample. Valves used to control the measuring procedure were computer controlled

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using HP-VEE program and servo motor PPN2 (Ekorex, Czech Republic). The pressure was measured by a capacitance diaphragm absolute gauge MKS Baratron type 690A11TRA. Measuring range of the gauge is from 0.1 Pa to 1333 Pa, accuracy stated by the manufacturer is 0.05 % of the reading. The sensor temperature was kept at 318 K, which constrained the upper temperature limit of the vapor pressure measurement to 313 K. Calibration of the pressure gauge at 318 K performed by the manufacturer at 11 equally spaced pressures from (0 to 1300) Pa with a maximum deviation of 0.03 %, is traceable to the National Institute of Standards and Technology (NIST). [Calibration was performed using MKS transfer standard S/N: 96120251A, which is calibrated with a CEC Air Deadweight tester, traceable to NIST.] Naphthalene was the first sample measured with this new apparatus. This eliminated any systematic error due to adsorption on internal walls of the tubing or contamination by traces of a compound that had been measured in the apparatus in a preceding experiment. The pressure gauge was connected to a signal conditioner MKS 670B, which displayed the pressure to nearest 0.01 Pa.

The pressure gauge MKS Baratron was connected to a stainless steel container with the measured material immersed in a Lauda RK 8 CP thermostat that allowed adjustment of the sample temperature in the temperature range from 223 K up to 473 K with stability better than 0.02 K. Sample temperature was measured by a platinum resistance thermometer Burns Engineering 12001-A-12-6-2-A in a four-wire connection calibrated by the manufacturer at the ice point and/or by comparison to standard platinum resistance thermometer (SPRT). This SPRT was calibrated to the ITS-90, and its calibration was traceable to NIST. The uncertainty of the measurement of sample temperature was 0.02 K, which is insignificant in the pressure range investigated in this work.

The uncertainty in the pressure measurements is adequately described by the expression

$$\sigma(p/\text{Pa}) = 0.005(p/\text{Pa}) + 0.05 \qquad (1)$$

Prior to measurement of vapor pressure, the apparatus was checked for tightness by MKS PICO vacuum leak detector (MKS Instruments Inc., USA). The apparatus was evacuated between individual measurement cycles by a turbomolecular pump to a pressure of about 10^{-5} Pa. A computer using the HP-VEE program monitored the temperature and pressure of the sample and controlled the measuring procedure. Experiments were carried out in the given temperature interval by varying temperature at random.

Adsorption of vapors of the measured sample on internal walls of the apparatus can be a significant source of systematic errors when using a static method. We reduced the possibility of adsorption by using electrochemically polished tubing, by keeping the internal surface of the apparatus as small as possible and by using a turbomolecular pump (Pfeiffer Vacuum TSH071). The use of a turbomolecular pump instead of a rotary and/or a diffusion pump ensures that oil from a rotary or a diffusion pump will not form a film on the inner surface of the apparatus; the oil film enables adsorption of vapors of the measured compound.

Systematic errors can be caused also by thermal transpiration. This phenomenon was determined experimentally, as described later.

Results and Discussion

Measured Vapor Pressure of Solid Naphthalene. Results of our measurements are given in Table 1. Vapor pressures were also measured below 0.1 Pa in order to explore capabilities of our apparatus; these values were not considered when developing recommended data.

Thermal Transpiration. Thermal transpiration can significantly influence measurements of vapor pressure in a static apparatus. As literature results of studies devoted to thermal transpiration are not conclusive and because of some misprints in original papers, we found it desirable to briefly summarize the current status of this topic.

Thermal transpiration occurs in an experimental setup where the pressure gauge is kept at a higher temperature than the sample vessel. This arrangement, which is conventional for most static apparatuses described in the literature (for example, refs 1 and 9−12), avoids condensation of sample vapors in the system tubing as well as in the pressure gauge itself. In addition, in the case of frequently used capacitance diaphragm gauges (CDG), which are sensitive to temperature changes, it improves the stability of the pressure reading. The phenomenon of thermal transpiration can result in the pressure p_2 read by the pressure gauge at temperature T_2 to be higher than the pressure p_1 in the sample vessel kept at a lower temperature T_1. The influence of thermal transpiration, i.e., the value of the ratio p_2/p_1, depends on several factors: on the Knudsen number $Kn = \lambda/d$, where λ is the mean free molecular path of measured sample, d is the diameter of tubing connecting the pressure gauge and sample vessel; on the ratio of temperatures, T_2/T_1; and on the tubing material connecting the pressure gauge to the sample vessel. For $Kn \ll 1$ (hydrodynamic region) the ratio p_2/p_1 is equal to unity, $p_2/p_1 = 1$, for $Kn \gg 1$ (molecular region) the ratio p_2/p_1 is equal to the limiting value $p_2/p_1 = \sqrt{T_2/T_1}$. [This limiting value is valid for apertures only not for tubing as was found by refs 21, 32, 124, and 125]. These experimental results show that the limiting value should be equal to approximately $(T_2/T_1)^{0.4}$. Between these extreme cases there is the so-called transitional regime, and the ratio p_2/p_1 lies between unity and the limiting value, $1 < p_2/p_1 < \sqrt{T_2/T_1}$.

Vapor pressure measurements by a static method are usually performed either in the hydrodynamic (higher pressures) or in the transitional regime. In the transitional regime the measured pressure is often quite low and close to the limit of practicability of performing measurement of vapor pressure by a static method. For calculation of the ratio p_2/p_1 in the transitional regime, several relationships can be found in the literature: Weber equation[13] (as cited, e.g., by ref 14); Weber-Schmidt equation;[15] Kavtaradze equation;[16] Miller equation;[17] Kanki et al. equation;[18] Liang equation[19] and its modifications;[20,21] Takaishi and Sensui equation[22] and its modification;[23] and the Šetina equation.[24] Besides these empirical or semiempirical equations, theoretical data based on the solution of the Boltzmann equation reported by Sharipov and Seleznev[25] can be used for calculation of the influence of thermal transpiration.

Generally, all these equations (except the Kavtaradze equation[16]) required as input information the diameter (d) of the tubing connecting the pressure gauge and sample vessel, pressure p_2 read by the gauge, temperatures T_1 and T_2 and, in addition, also the dynamic viscosity or collision diameter of the measured gas. For organic compounds, the dynamic viscosity of the gas is not usually available and must be estimated by a suitable method (see, e.g., Poling et al.[26]). It is important to note that all equations except for the modification of Takaishi and Sensui equation[23] were derived from the measurements on inorganic gases only. Data reported by Sharipov and Seleznev[25] are valid for

Table 1. Experimental Data on Vapor Pressure of Solid Naphthalene

T/K	$p_{\mathrm{sat}}^{\mathrm{exp}}$/Pa	$(p_{\mathrm{sat}}^{\mathrm{exp}} - p_{\mathrm{sat}}^{\mathrm{calc}})^a$/Pa	$100 \cdot (p_{\mathrm{sat}}^{\mathrm{exp}} - p_{\mathrm{sat}}^{\mathrm{calc}})/p_{\mathrm{sat}}^{\mathrm{calc}}$	T/K	$p_{\mathrm{sat}}^{\mathrm{exp}}$/Pa	$(p_{\mathrm{sat}}^{\mathrm{exp}} - p_{\mathrm{sat}}^{\mathrm{calc}})^a$/Pa	$100 \cdot (p_{\mathrm{sat}}^{\mathrm{exp}} - p_{\mathrm{sat}}^{\mathrm{calc}})/p_{\mathrm{sat}}^{\mathrm{calc}}$
258.48	0.11	−0.008	−7.0	278.49	1.38	0.005	0.3
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258.48	0.11	−0.008	−7.0	278.49	1.38	0.005	0.3
258.48	0.11	−0.008	−7.0	278.49	1.39	0.015	1.1
258.49	0.11	−0.008	−7.1	278.49	1.39	0.015	1.1
258.49	0.11	−0.008	−7.1	278.49	1.38	0.005	0.3
258.49	0.11	−0.008	−7.1	278.49	1.36	−0.015	−1.1
258.49	0.11	−0.008	−7.1	278.49	1.37	−0.005	−0.4
263.48	0.22	−0.007	−2.9	278.49	1.38	0.005	0.3
263.48	0.22	−0.007	−2.9	278.49	1.37	−0.005	−0.4
263.48	0.22	−0.007	−2.9	283.49	2.41	0.012	0.5
263.48	0.22	−0.007	−2.9	283.49	2.41	0.012	0.5
263.49	0.23	0.003	1.4	283.49	2.41	0.012	0.5
263.49	0.23	0.003	1.4	288.49	4.11	0.013	0.3
263.49	0.23	0.003	1.4	288.49	4.10	0.003	0.1
263.49	0.23	0.003	1.4	288.49	4.10	0.003	0.1
268.48	0.42	−0.003	−0.7	293.49	6.88	0.015	0.2
268.48	0.41	−0.013	−3.1	293.49	6.88	0.015	0.2
268.48	0.43	0.007	1.6	293.49	6.88	0.015	0.2
268.48	0.42	−0.003	−0.7	298.49	11.40	0.098	0.9
273.48	0.78	0.009	1.2	298.49	11.40	0.057	0.5
273.48	0.77	−0.001	−0.1	298.49	11.30	0.046	0.4
273.48	0.78	0.009	1.2	298.49	11.40	0.057	0.5
273.48	0.78	0.009	1.2	298.49	11.30	0.046	0.4
273.49	0.78	0.008	1.1	303.50	18.30	0.048	0.3
273.49	0.77	−0.002	−0.2	303.50	18.30	−0.013	−0.1
273.49	0.78	0.008	1.1	303.50	18.20	−0.044	−0.2
273.49	0.78	0.008	1.1	303.50	18.30	−0.024	−0.1
273.68	0.80	0.011	1.3	303.50	18.20	−0.044	−0.2
273.68	0.81	0.021	2.6	308.51	29.00	−0.067	−0.2
273.68	0.80	0.011	1.3	308.51	29.00	0.099	−0.3
273.68	0.81	0.021	2.6	308.51	29.00	−0.107	−0.4
273.68	0.80	0.011	1.3	308.51	29.00	−0.099	−0.3
273.68	0.81	0.021	2.6	313.52	45.40	−0.150	−0.3
278.48	1.37	−0.004	−0.3	313.52	45.40	−0.091	−0.2
278.48	1.38	0.006	0.5	313.52	45.40	−0.114	−0.3
278.48	1.37	−0.004	−0.3	313.52	45.50	−0.073	−0.2
278.48	1.37	−0.004	−0.3				

[a] $p_{\mathrm{sat}}^{\mathrm{calc}}$ vapor pressure calculated from the Cox eq 9 with parameters from Table 6.

monatomic gases only even though they can be used for polyatomic gases in some cases.

We evaluated the effect of thermal transpiration by selecting helium as a test compound and concluded that all equations except the Kavtaradze equation[16] are capable of reasonably describing the experimental data on thermal transpiration obtained for inorganic gases. For inorganic gases, the data on dynamic viscosity are generally available. This declines the uncertainty in prediction of thermal transpiration caused by inaccurate estimation of dynamic viscosity of the gas. In many cases, however, a modification of relations was necessary to achieve better agreement between calculated and experimental values (see, for example, refs 21, 27, and 28). In addition, some authors testing the above-mentioned equations presented an opposite assessment of published relationships. The equation, which described well experimental data obtained for one apparatus, often failed for another apparatus. It seems that no equation is generally capable of predicting the influence of thermal transpiration; the influence of thermal transpiration must be tested and determined for each apparatus experimentally. Furthermore, authors correcting their results for thermal transpiration should provide either both uncorrected and corrected data or supply all information that is necessary for obtaining uncorrected data. This will enable a new correction after a generally applicable model for thermal transpiration is found.

It is also worthwhile to note that we found some typing and other errors in the literature dealing with thermal transpiration. The publication by Poulter et al.,[29] which has been widely cited, contains a wrong relationship for parameter $X = 0.133 p_2 d$ (eq 4 in ref 29); it should read $X = 7.5 p_2 d$, when entering pressure p_2 in Pascal and diameter d in meters. In the same paper, in eq 7 the collision diameter calculated from viscosity data using the Lennard−Jones 12:6 potential should be employed instead of the equivalent elastic sphere diameter derived by Kennard.[30] Takaishi and Sensui[22] used a misleading expression "exp[0.507D]" and "exp[0.607D]“ in eqs 9 and 10 where parameters of Takaishi and Sensui equation are to be computed from the collision diameter. Surprisingly, "exp" does not mean a natural number root but a decimal root. Equations 9 and 10 should read "$10^{0.507D}$" and "$10^{0.607D}$". These misleading expressions led to incorrect assessment of prediction capability of the Takaishi and Sensui equation (for example, in ref 31).

For the above reasons, we performed the measurement of thermal transpiration experimentally during vapor pressure measurement of naphthalene. An apparatus similar to that described above was used; the length of the tubing was comparable, but a differential pressure gauge MKS Baratron 616A11TRC-S was used, which can be heated to 573 K. Sample was kept at constant temperature T_1 = 283.48 K (vapor pressures was about 2.7 Pa). The temperature of the pressure gauge T_2 was changed from 323.15 K where no effect of thermal transpiration should have been observed up to 473.15 K, where effect of thermal transpiration should have been detectable. However, no difference in pressure p_2 with increase in temperature T_2 was observed (i.e., thermal transpiration of naphthalene was negligible or lower than the resolution of our pressure gauge, which is equal to 0.01 Pa). This observation was in accordance with the Takaishi and Sensui equation,[22] which is recommended by Poulter et al.[29] and by Jitschin and Röhl[32] for correction of thermal transpiration when using capacitance diaphragm gauges.

Data Correlation. There are exact thermodynamic relations between vapor pressure (p_{sat}), enthalpy of vaporization ($\Delta_{\mathrm{l}}^{\mathrm{g}} H_{\mathrm{m}}$), and difference between heat capacities of the gaseous and liquid phases ($\Delta_{\mathrm{l}}^{\mathrm{g}} C_{p,\mathrm{m}}^0$). King and Al-Najjar[33] suggested simultaneous correlation of the above properties. This idea was followed by other investigators who noticed the advantage of this approach, namely, that properties included in the correlation are thermodynamically related.[34−37] Moreover, the resulting vapor pressure equation is valid over the combined temperature ranges of all these properties. The method was thoroughly tested in our laboratory,[38] applied to the development of recommended vapor pressure of several liquid compounds,[39−42] and extended also to solid−vapor equilibria.[43−45]

Vapor pressure (p_{sat}), enthalpy of vaporization ($\Delta_{\mathrm{l}}^{\mathrm{g}} H_{\mathrm{m}}$) or enthalpy of sublimation ($\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}$), and the difference between perfect gas heat capacity and heat capacity of liquid $\Delta_{\mathrm{l}}^{\mathrm{g}} C_{p,\mathrm{m}}^0 = C_p^{\mathrm{g}0} - C_p^{\mathrm{l}}$ (or heat capacity of solid $\Delta_{\mathrm{s}}^{\mathrm{g}} C_{p,\mathrm{m}}^0 = C_p^{\mathrm{g}0} - C_p^{\mathrm{s}}$) are linked by exact thermodynamic relationships:

$$RT^{2}(\mathrm{d}\ln p/\mathrm{d}T)_{\mathrm{sat}} = \Delta_{\mathrm{cd}}^{\mathrm{g}} H_m/\Delta_{\mathrm{cd}}^{\mathrm{g}} Z = \Delta H' \tag{2}$$

$$(\mathrm{d}\Delta H'/\mathrm{d}T)_{\mathrm{sat}} = R[\mathrm{d}\{T^2(\mathrm{d}\ln p/\mathrm{d}T)\}/\mathrm{d}T]_{\mathrm{sat}} = \Delta C' = \Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0 + [\mathrm{pVT\ correction}] \tag{3}$$

here subscript "sat" denotes a derivative along the saturation line, $\Delta_{\mathrm{cd}}^{\mathrm{g}} H_{\mathrm{m}}$ stands for vaporization or sublimation enthalpy, $\Delta_{\mathrm{cd}}^{\mathrm{g}} Z$ stands for the difference between the compressibility factors of the coexisting phases, $\Delta H'$ and $\Delta C'$ are auxiliary quantities that can be calculated using eq 2 and eq 3 either from the vapor pressure correlating equation (by substituting the derivative d ln p/dT into eq 2 and 3) or from experimental values of enthalpy of vaporization ($\Delta_{\mathrm{l}}^{\mathrm{g}} H_{\mathrm{m}}$) or enthalpy of sublimation ($\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}$) and $\Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0$ calculated from experimental data by combining spectroscopic values of heat capacity of perfect gas ($C_p^{\mathrm{g}0}$) and calorimetric values of heat capacity of liquid (C_p^{l}) or heat capacity of solid (C_p^{s}). The possibility to calculate $\Delta H'$ and $\Delta C'$ both from the experimental thermal data and vapor pressure data and from a vapor pressure correlating equation means that after selecting a suitable relationship describing p_{sat} versus T it is possible to correlate simultaneously experimental vapor pressures (p_{sat}), enthalpies of vaporization ($\Delta_{\mathrm{l}}^{\mathrm{g}} H_{\mathrm{m}}$) or enthalpies of sublimation ($\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}$), and heat capacity difference ($\Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0$) as a function of temperature.

In principle, any vapor pressure equation can be used for such type of correlation. It should be noted, however, that the simplest equation, obtained from the Clapeyron equation assuming enthalpy of vaporization/sublimation is constant

$$\ln(p_{\mathrm{sat}}/\mathrm{Pa}) = A - \frac{B}{T/\mathrm{K}} \tag{4}$$

implies that heat capacity difference is zero and cannot be used for the simultaneous correlation. This equation is frequently used when the temperature range is narrow and/or scatter of vapor pressure data is large. The Antoine equation

$$\ln(p_{\mathrm{sat}}/\mathrm{Pa}) = A - \frac{B}{T/\mathrm{K} + C} \tag{5}$$

was shown not to be flexible enough to describe simultaneously all input data, vapor pressure, enthalpy of vaporization, and heat capacity difference.[38] Other equations have also been used for description of vapor pressure of solid naphthalene: a four-term Chebyshev polynomial[1] and a five-term polynomial in reciprocal temperature.[7] The Clarke and Glew equation[46]

$$R\ln\frac{p_{\mathrm{sat}}}{p^0} = -\frac{\Delta_{\mathrm{cd}}^{\mathrm{g}} G_{\mathrm{m}}^0(T_{\mathrm{mean}})}{T_{\mathrm{mean}}} - \Delta_{\mathrm{cd}}^{\mathrm{g}} H_{\mathrm{m}}^0(T_{\mathrm{mean}}) \times \left(\frac{1}{T_{\mathrm{mean}}} - \frac{1}{T}\right) + \Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0(T_{\mathrm{mean}})\left(\frac{T_{\mathrm{mean}}}{T} - 1 + \ln\left(\frac{T}{T_{\mathrm{mean}}}\right)\right) + \left(\frac{T_{\mathrm{mean}}}{2}\right)\left(\frac{\partial \Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0}{\partial T}\right)(T_{\mathrm{mean}})\left(\frac{T}{T_{\mathrm{mean}}} - \frac{T_{\mathrm{mean}}}{T} - 2\ln\left(\frac{T}{T_{\mathrm{mean}}}\right)\right) + \ldots \tag{6}$$

was extensively used by the group at the University of Utrecht (for more detailed explanation and meaning of symbols see, for example, refs 9 and 47). The advantage of this equation lies in a physical meaning of the fitted parameters. Very often this equation was used in a truncated form with three parameters (i.e. $\Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0$, difference between heat capacity of perfect gas and that of a condensed phase "cd" is constant) or two parameters (i.e., $\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}$ or $\Delta_{\mathrm{l}}^{\mathrm{g}} H_{\mathrm{m}}$ is constant and $\Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0$ is zero).

The Wagner equation[48] is very popular for fitting vapor pressures of liquids, but it cannot be used for fitting vapor pressure of solids as it is constrained to the critical point. Another way to derive a vapor pressure equation is to start from temperature dependence of $\Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0$. When a quadratic equation is adequate

$$\Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0/R = a + b(T/\mathrm{K}) + c(T/\mathrm{K})^2 \tag{7}$$

then the vapor pressure equation has the form

$$\ln(p_{\mathrm{sat}}/\mathrm{Pa}) = A\ln(T/\mathrm{K}) + B(T/\mathrm{K})^{-1} + C + D(T/\mathrm{K}) + E(T/\mathrm{K})^2 \tag{8}$$

Parameter E is equal to 0 when the temperature dependence of $\Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0$ is linear.

The Cox equation[49] has the form

$$\ln\frac{p_{\mathrm{sat}}}{p^0} = \left(1 - \frac{T^0/\mathrm{K}}{T/\mathrm{K}}\right)\exp\left(\sum_{i=0}^{n} A_i (T/\mathrm{K})^i\right) \tag{9}$$

with T^0 and p^0 being temperature and pressure of an arbitrarily chosen reference point. $n = 2$ is usually used; less or more parameters can be used when the temperature range is too narrow or too wide or when the temperature dependence of $\Delta_{\mathrm{cd}}^{\mathrm{g}} C_{p,\mathrm{m}}^0$ is complex. The Cox equation was found[38] to be the most adequate for describing simultaneously vapor pressure and related thermal data as a function of temperature down to and below the triple point.

The parameters of the Cox equations were calculated in this work by the simultaneous correlation of experimental vapor pressures, differences in experimental heat capacities in the solid phase and heat capacities of the perfect gas, and experimental enthalpies of sublimation. The thermodynamic background for the temperature correlation of vapor pressure and the related thermal data, hereafter denoted as the SimCor method, has been described in the literature.[50,51] By using exact thermodynamic relationships, the SimCor method combines properties determined by different experimental techniques that usually cover different temperature ranges and allows a consistent description of the (vapor + liquid) and the (vapor + solid) saturation curve. The SimCor method helps to reveal systematic errors in input data and can also serve for the qualified estimation of missing data, in particular enthalpies of vaporization and/or enthalpies of sublimation. In addition, the SimCor method is often used for a controlled extrapolation of medium-pressure range vapor pressures down to or below the triple point.

Vapor Pressure of Liquid Naphthalene. The most recent comprehensive work devoted to selection of the recommended vapor pressures of liquid naphthalene is that by van der Linde et al.[47] They selected three ebulliometric sets, two published by Ambrose et al.[52] and one published by Chirico et al.[7] Chirico et al.[7] discussed and explained small difference between their data and two data sets by Ambrose et al.[52] In this work we follow conclusions of Chirico et al.[7] because our calculations showed better consistency of the data by Chirico et al.[7] with the differences in heat capacities $\Delta_{\mathrm{l}}^{\mathrm{g}} C_{p,\mathrm{m}}^{0}$.

Some new papers reporting the vapor pressure of liquid naphthalene have appeared since the paper by Chirico et al.[7] The new data do not change the value of the vapor pressure at the triple point (which plays a crucial role in our calculations, see next parts) either because of higher data uncertainty (Guetachew et al.[53]) or because they cover a high-temperature region only.[54−56]

Preliminary Fit. The number of papers reporting results for vapor pressure of solid phase naphthalene is large, and questions arise as how to compare all these data sets clearly and lucidly. For many years it was common to plot ln p_{sat} as a function of $1/T$. Such type of plot is rather insensitive to errors between and within data sets, and even large differences look “acceptable”. Another way is to present data in the form of a deviation plot that displays absolute or relative difference in pressure of a given data set with respect to a selected reference data set as a function of temperature. Disadvantage of such plots is that 10 % difference, quite acceptable for pressures well below 1 Pa, is not acceptable at say 10 kPa or 100 kPa. If a wide pressure range is to be displayed in a deviation plot, the plot should be divided into several sections (e.g., as in the papers by Ambrose et al.[57] or Wexler[58]). Wilsak and Thodos[59] suggested to transform plot of ln p_{sat} as a function of $1/T$ into some other quantities, which would make the differences between data sets as well as scatter of the data more apparent than in the original plot. A similar approach was used by Oonk et al.[60] and by van Genderen and Oonk,[61] who suggested to scale vapor pressures and to plot $\ln f = \ln p_{\mathrm{sat}} - \alpha + \beta/T$ as a function of $1/T$.

None of the above-mentioned approaches helps to select the “true” or the most acceptable data if several sets that are subject to a similar experimental uncertainty are being compared. In addition, the above-mentioned approaches are based on a graphical comparison of vapor pressure data and do not make use of exact thermodynamic relationships that exist between vapor pressure and related thermal data.

In this work, we used a different approach: a preliminary multi-property regression based on independently measured properties was performed using the following data: temperature and the corresponding vapor pressure at the triple point, enthalpy of sublimation at the triple point, and difference in heat capacities of solid and of perfect gas. Papers reporting vapor pressure of solid naphthalene were grouped on the basis of experimental techniques used, and data reported therein were compared with the result of the preliminary correlation. Data used for the preliminary correlation as well as the results of the correlation are outlined below.

Triple Point. Temperature of the triple point, 353.37 K (in ITS-90), was taken from Chirico et al.[8] The vapor pressure at the triple point temperature, 993.5 Pa, was calculated from the fit of liquid vapor pressures by the Wagner equation (see Table 7 in ref 7) developed by Chirico et al.[7]

Enthalpy of Sublimation at the Triple Point. In the literature, two principle ways are described for determining the enthalpy of sublimation of naphthalene: from sublimation pressures or calorimetrically (see also sections ”Enthalpies of Sublimation” in “Final Correlation, Data Sources” for a more detailed account). In the preliminary fit it was not known which sets of data on vapor pressure of solid naphthalene and of calorimetrically determined enthalpy of sublimation were mutually consistent. We therefore derived the enthalpy of sublimation at the triple point temperature from recommended values of the enthalpy of fusion and the enthalpy of vaporization at the triple point temperature 353.37 K.

The enthalpy of fusion $\Delta_{\mathrm{s}}^{\mathrm{l}} H_{\mathrm{m}}(353.37\ \mathrm{K}) = (18.993 \pm 0.019)\ \mathrm{kJ{\cdot}mol^{-1}}$ was taken from Chirico et al.,[8] who compared their experimental value with previously published values. The enthalpy of vaporization $\Delta_{\mathrm{l}}^{\mathrm{g}} H_{\mathrm{m}}(353.37\ \mathrm{K}) = (51.39 \pm 0.17)\ \mathrm{kJ{\cdot}mol^{-1}}$ was derived from vapor pressure by Chirico et al.[7] as calorimetric values measured near the triple point temperature are not reliable. These values were obtained by differential scanning calorimetry,[62−64] but the temperature of measurement is either given as a broad temperature range or not reported at all. The remaining published values of enthalpy of vaporization at the triple point temperature were obtained by gas chromatography for subcooled liquid at 298.15 K and converted to the triple point temperature.[65−67] Due to this conversion we treat them as indirect data, which we do not include into calculations in this work.

The enthalpy of vaporization measured by a flow apparatus (Barrow and McClellan[68]), which is in excellent agreement with value derived from vapor pressures by Chirico et al.,[7] was measured at 440.9 K. Its conversion to triple point temperature would be associated with higher uncertainty than derivation of $\Delta_{\mathrm{l}}^{\mathrm{g}} H_{\mathrm{m}}$ from vapor pressure data.

PVT corrections used in calculations of $\Delta_{\mathrm{l}}^{\mathrm{g}} H_{\mathrm{m}}$, which amounts to 1.7 % at 440.9 K (vapor pressure equal to 27.9 kPa) and to 0.2 % at the triple point temperature, was evaluated from the virial equation with second virial coefficient estimated by method of Tsonopoulos.[69] Critical parameters needed in this method were selected by Chirico et al.[7] from the measurements by Ambrose et al.;[70] densities at saturation pressure, which play a negligible role in the PVT correction calculations, were taken from Chirico et al.[7]

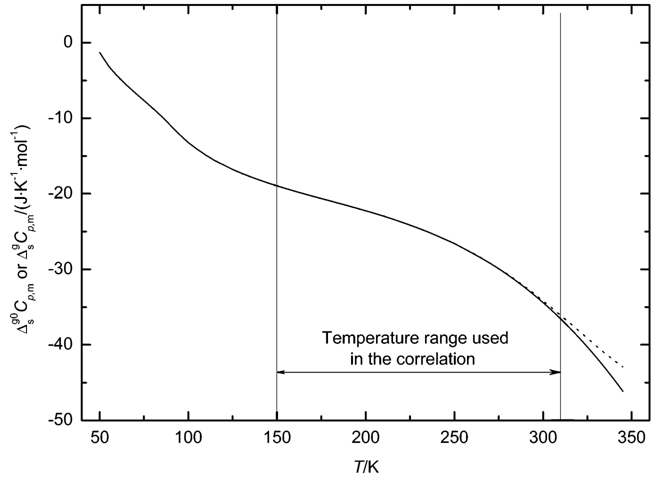

Figure 2. Temperature dependence of $\Delta_s^g C^0_{p,m}$ and $\Delta_s^g C_{p,m}$. $C^0_{p,m}$ taken from Frenkel et al.[72] $C^s_{p,m}$ taken from Chirico et al.[8] —, $\Delta_s^g C^0_{p,m} = C^{g0}_{p,m} - C^s_{p,m}$; ···, $\Delta_s^g C_{p,m} = C^g_{p,m} - C^s_{p,m}$.

Table 2. Parameters of the Cox Eq 9 from the Preliminary Fit

A_0	A_1	A_2	T^0 / K	p^0 / Pa
3.272356	$-2.659109 \cdot 10^{-4}$	$-4.347265 \cdot 10^{-9}$	353.37	993.5

The above-mentioned values of $\Delta_s^l H_m$ and $\Delta_l^g H_m$ yield enthalpy of sublimation at the triple point equal to (70.38 ± 0.17) kJ·mol^{-1}.

Differences in Solid and Perfect Gas Heat Capacities. Perfect gas heat capacities of naphthalene calculated from experimental vibrations by Chen et al.[71] and fitted by a nonlinear equation by Frenkel et al.[72] were used in this work. Solid heat capacities of naphthalene were taken from Chirico et al.[8]

Differences in heat capacities of the perfect gas and those of solid as a function of temperature are shown in Figure 2. $\Delta_s^g C^0_{p,m}$ is not a linear function of temperature; therefore, a vapor pressure equation with more than two adjustable parameters should be used. We found out that for our preliminary correlation it was essential that an almost linear part of the curve $\Delta_s^g C^0_{p,m} = f(T)$ was included in the fit (i.e., $\Delta_s^g C^0_{p,m}$ approximately from $T_{\min} = 150$ K to $T_{\max} = 310$ K). Change of the upper limit of the $\Delta_s^g C^0_{p,m}$ data by ± 30 K (i.e., $T_{\max} = 280$ K or $T_{\max} = 340$ K) had no significant effect on the calculated vapor pressures and enthalpies of sublimation. For example, the difference in vapor pressure at 200 K, when the upper limit of $\Delta_s^g C^0_{p,m}$ was changed from 310 K to 340 K, was less than 4 % (which is equal to $2 \cdot 10^{-7}$ Pa) and was smaller at higher temperatures. For the same change of the upper limit of $\Delta_s^g C^0_{p,m}$ the difference in $\Delta_s^g H_m$ was smaller than 0.2 kJ·mol^{-1} over the whole temperature range from 150 K to the triple point temperature.

Parameters of the Vapor Pressure Equation. Equation 8 with five adjustable parameters as well as the Cox eq 9 with the fixed reference point $T^0 = T_{tp}$ and $p^0 = p_{tp}$, where T_{tp} and p_{tp} is the temperature and pressure of the triple point, and three and four adjustable parameters yielded very similar results. Therefore, the equation with the smallest number of parameters (the Cox equation with the three parameters) was used. Its parameters are given in Table 2.

Final Correlation, Data Sources. In this section we present and discuss literature data, grouped according to experimental techniques, and select data for the final multi-property correlation of vapor pressure, enthalpy of sublimation, and difference in heat capacity of perfect gas and that of solid. Only data published after 1950 are considered because older data were shown by Ambrose at al.[1] and by Chirico et al.[7] to be in error.

Reported temperatures were converted to ITS-90; it should be noted that the largest difference (at the triple point, 353.37 K) is 0.027 K, which represents a difference in vapor pressure of 1.8 Pa (i.e., 0.18 %). At lower temperatures the influence of the temperature scale on vapor pressures rapidly decreases, and below 320 K differences between temperatures in the original scale and that in ITS-90 are insignificant.

Authors in most cases did not report which temperature scale was used. In such cases data published before 1970 were assumed to adhere to ITS-48, data published from 1970 to 1991 adhered to IPTS-68, and data from 1992 onward adhered to ITS-90. A summary of the existing data is presented in Table 3.

Vapor Pressure of Solid Naphthalene. Data on vapor pressure of solid naphthalene in the literature are abundant. Review papers by Delle Site,[73] Shiu and Ma,[74] and Chickos and Acree[75] cover most of the sources of existing data. Delle Site[73] also described the main features and limitations of different methods used for vapor pressure measurements. Therefore, only short comments to respective methods are presented below.

Static Method. Results obtained by the static method belong to the most accurate and usually cover a wide pressure range, usually from 1 Pa to 10 kPa. Possible sources of systematic errors are sample impurities, incomplete degassing (resulting in a higher value of the measured vapor pressure than the true value), adsorption on internal walls of the apparatus (resulting in a lower value of vapor pressure), and in measurements of vapor pressure below 10 Pa, in some special arrangements, also thermal transpiration.

Fowler et al.[76] used a sealed quartz helix. All remaining static measurements were performed using apparatuses of basically similar construction that differ mainly in the pressure gauges they employed. Ambrose et al.[1] and de Kruif et al.[10] used a Baratron 170M, de Kruif et al.[9] used a MKS 94AH, van Ekeren et al.[77] used a spinning-rotor friction gauge, Sasse et al.[11] and Guetachew et al.[53] used a Datametrics 1173, and Guetachew et al.[53] used a Rosemount gauge (unspecified model) for pressures above 3 kPa. Though most of the above-mentioned measurements appear to be done very carefully and thoroughly, mutual agreement between different measurements is not satisfactory.

Fowler et al.,[76] de Kruif et al.,[9] Sasse et al.,[11] and Guetachew et al.[53] measured also vapor pressures of liquid naphthalene. We used these data and compared them with the recommended data by Chirico et al.[7] in order to estimate the overall reliability of data by the particular authors.

Results reported by Fowler et al.[76] in the liquid phase are slightly higher than the recommended values by Chirico et al.[7] With the exception of one data point, deviations are smaller than 1 %; absolute deviations are within 20 Pa (Fowler et al.[76] reported precision of measurements 4 Pa for pressures up to 13 kPa).

Absolute deviations in vapor pressures of solid naphthalene (see Figure 3) reported by Fowler[76] are smaller than 15 Pa, and with two exceptions vapor pressures are higher than those calculated from the preliminary fit (maximum percentage error being about 5 %). All data points were

Table 3. Sources of Vapor Pressure Data for Solid Naphthalene

reference	N^a	$T_{\min}$/K	$T_{\max}$/K	σ_T/K	σ_p	purity/%	method
Bradley and Cleasby[103]	11	280	294	nosp.	nosp.	nosp.	eff
Sherwood and Bryant[78]	S	273	311	nosp.	nosp.	nosp.	sat
Hoyer and Peperle[94]	S	253	283	nosp.	nosp.	nosp.	eff
Sklyarenko et al.[95]	S	293	303	nosp.	nosp.	nosp	eff
Aihara[106]	5	276	283	nosp.	nosp.	nosp.	visc
Gil′denblat et al.[79]	28	289	323	0.05	nosp.	nosp.	sat
Miller[2]	4	226	263	nosp.	5 %	99.7	eff
Fowler et al.[76]	12	313	352	0.01	4 Pa	99.99	sta
Karyakin et al.[96]	S	283	323	0.05	3 %	99.8	eff
Lukashenko and Pogadaev[97]	5	243	323	0.1	3 %	nosp.	eff
Baskakov and Suprun[80]	S	298	343	0.25	nosp.	nosp.	sat
Radchenko[98]	S	283	323	nosp.	nosp.	nosp.	eff
McEachern and Sandoval[107]	4	281	290	nosp.	nosp.	99.95	eva
Radchenko and Kitaigorodskii[104]	9	282	297	nosp.	2.2 %	nosp.	eff
Sinke[3]	1	275		nosp.	2 %	99.99	sat
Ambrose et al.[1]	22	264	343	0.01	2 %	99.95	sta
Clark[88]	H	302	329				sat
Chickos[108]	S	263	293	0.2	nosp.	nosp.	hs
de Kruif and van Ginkel [91], de Kruif[92]	S	253	273	0.1	nosp.	nosp.	eff
Macknick and Prausnitz [90]	6	280	305	0.05	nosp.	99+	sat
de Kruif et al. [10]	14	274	293	0.01	1.5 %	nosp.	sta
de Kruif et al.[9]	67	274	353	0.01	6 Pa	99.97	sta
Colomina et al.[105]	8	271	285	0.005	nosp.	99.95	eff
Glukhova et al.[99]	H	293	331	nosp.	nosp	nosp.	eff
Grayson and Fosbraey[85]	6	302	352	nosp.	nosp.	nosp.	sat
van Ekeren et al.[77]	10	244	256	0.01	4 %	99.97	sta
Sonnefeld et al.[89]	S	283	323	0.05	5 %	nosp.	sat
Mironov and Khudyakov[87]	7	294	304	0.1	6 %	nosp.	sat
Glukhova et al.[100]	H	293	331			nosp.	eff
Matsubara and Kuwamoto[81]	H	333	353			nosp.	sat
Sato et al. [82]	11	299	331	0.06	3 %	98	sat
Sakoguchi et al. [83]	3	323	343	nosp.	0.5 %	nosp.	sat
Khudyakov [113]	S	337	352	nosp.	nosp.	nosp.	chro
Sasse et al. [11]	17	261	343	0.02	2 %	99	sta
Wania et al. [84]	7	243	273	0.01	nosp.	nosp.	sat
Guetachew et al. [53]	14	264	353	0.02	2 %	99	sta
Nass et al. [101]	E	298		nosp.	nosp.	99.9+	sat
Yasuoka et al. [86]	S	273	323	nosp.	nosp.	nosp.	sat
Niederfellner et al. [102]	E	298		nosp.	nosp.	nosp.	sat
Boller and Wiedemann [56]	8	267	303	nosp.	nosp.	nosp.	eff

[a] Number of points (S, eq only; E, extrapolated value; H, only sublimation enthalpy reported); σ_T, error in temperature; σ_p, error in pressure; nosp., not specified. Codes for method: chro, chromatographic; eff, effusion; eva, free evaporation; hs, headspace; sat, saturation; sta, static; visc, viscosity gauge.

measured at higher temperatures than in this work. We concluded that the Fowler et al.[76] data were the best at the time of their measurement, but they were superseded by newer investigations with smaller scatter and with more realistic temperature dependence of $\Delta_s^g H_m$ (see Figure 4) and $\Delta_s^g C_{p,m}^0$ (see Figure 5).

De Kruif et al.[9] reported values in the liquid phase, which are consistently lower than the recommended data by Chirico et al.[7] Maximal deviations are above −100 Pa (−2.7 %) at 385 K, scatter near this temperature being about 50 Pa. Their recommended triple point pressure at 353.30 K (at IPTS-68; 353.279 K at ITS-90) is (980 ± 3) Pa. This is in reasonable agreement with the recommended data for the liquid phase.[7] Differences in vapor pressures of de Kruif et al.[9] from the preliminary fit are positive over the most of the solid region (from 274 K to 346 K, see Figure 3) and negative just below the melting point, and also above it, yielding $\Delta_s^g H_m$ with a slope differing from that obtained from the preliminary fit (see Figure 4). Most of the values below 340 K are, however, in reasonable agreement (differences within 3 %) with the preliminary fit.

Sasse et al.[11] reported their lowest value in the liquid phase at temperature of 353.31 K (at IPTS-68; 353.289 K at ITS-90), which is below the triple point temperature 353.37 K reported by Chirico et al.[8] Vapor pressure at 353.31 K is by 20 Pa (2 %) lower than the extrapolated value from Chirico et al. [7] The data by Sasse et al.[11] seem to be less accurate than those published in the next paper from the University of Lyon,[53] which reports four values measured with a Datametrics 1173 pressure gauge. These four values in the liquid phase are by (7 to 10) Pa higher than the recommended value.[7] Above 3 kPa (above 381 K), measurements were performed with a "Rosemont" (unspecified model); absolute deviations of the values measured by Rosemont are considerably higher, but still in most cases within the claimed uncertainty of 0.3 %.

In the solid phase, of the two data sets reported by Jose and co-workers,[11,53] results from the second paper[53] are in better agreement with the preliminary fit. The maximum deviation of 5 % at 268 K represents an absolute deviation of 0.02 Pa; most values lie within 0.5 %. Values at the lowest temperatures tend to be too low; this trend was observed also with our measurements (see below).

The spinning-rotor friction gauge data by van Ekeren et al.[77] are consistently higher than those obtained from the preliminary fit, but relative deviations are only about (2 to 3) %, which can be regarded as a very good agreement in this pressure region (absolute deviations are below 10^{-3}

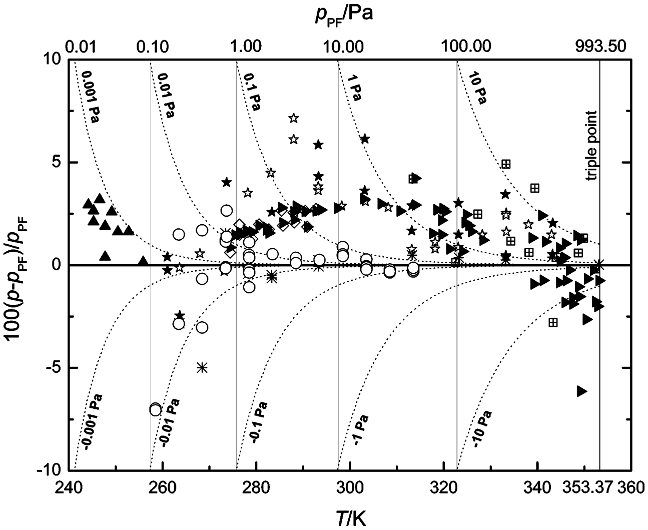

Figure 3. Static method. Deviation plot of vapor pressure data. p_{PF} is calculated from the Cox eq 9 with parameters obtained from preliminary fit (see Table 2). ○, this work; ⊞, Fowler et al.;[76] ☆, Ambrose et al.;[1] ◇, de Kruif et al.;[10] triangle right solid, de Kruif et al.;[9] ▲, van Ekeren et al.;[77] ★, Sasse et al.;[11] ∗, Guetachew et al.[53] ···, Absolute errors (0.001 Pa, 0.01 Pa, 0.1 Pa, 1 Pa, 10 Pa).

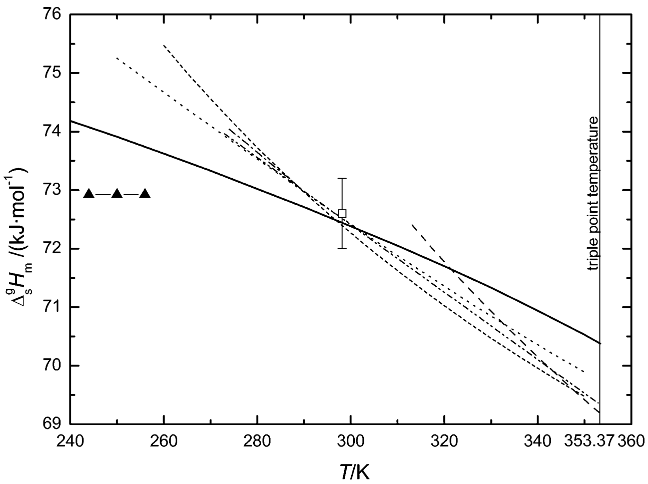

Figure 4. Static method. Comparison of $\Delta_s^g H_m$ calculated from the vapor pressure equations given by respective authors and from the preliminary fit. —, Preliminary fit; – –, Fowler et al.;[76] ···, Ambrose et al.;[1] -·-·-, de Kruif et al.;[10] -··, de Kruif et al.;[9] —▲—, van Ekeren et al.;[77] - - -, Sasse et al.;[11] □, Sabbah et al.[5] (T = 298.15 K).

Pa). Enthalpy of sublimation derived from the data is however different from $\Delta_s^g H_m$ obtained from the preliminary fit.

Researchers who carried out vapor pressure measurement by a static method in the arrangement where the temperature of the pressure gauge T_2 was higher than the temperature of the sample cell T_1[1,9,10] corrected their results for thermal transpiration using the Bennet and Tompkins modification of the Liang equation.[20] However, they did not present any specific information about the correction made, such as diameter of the tubings in the apparatus or collision diameter of the measured gas. For example, Ambrose et al.[1] only stated that the correction was 15 % at the lowest pressures, 0.5 % at 298 K, and negligible at higher temperatures. Ambrose et al.[1] and de Kruif et al.[9,10] published only corrected values of vapor pressures, which are now not possible to convert to uncorrected values due to the lack of necessary additional information as mentioned above. For these reasons low vapor pressures obtained by the static method have aditional uncertainty. Uncertainty arising from thermal transpiration are, however, close to the resolution of capacitance diaphragm gauges (i.e., 0.01 Pa).

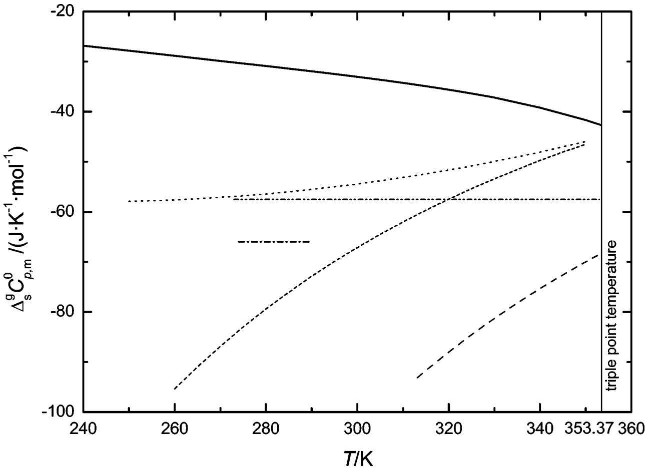

Figure 5. Static method. Comparison of $\Delta_s^g C_{p,m}^0$ calculated from the vapor pressure equations given by respective authors and from the preliminary fit. —, Preliminary fit; – –, Fowler et al.;[76] ···, Ambrose et al.;[1] ·-·-·, de Kruif et al.;[10] -··, de Kruif et al.;[9] - - -, Sasse et al.[11]

Ambrose et al.[1] stated that the uncertainty of their data was 2 % above 280 K and 5 % below that temperature. As can be seen from Figure 3, deviations are higher than this, particularly around 290 K. Values at lower temperature might be systematically influenced by inadequate correction for thermal transpiration.

Two sets of data reported by Jose and co-workers[11,53] were not corrected for thermal transpiration. Sasse et al.[11] stated that "generally only minor corrections for desorption had been made". No such corrections are mentioned by Guetachew et al.[53]

Note that $\Delta_s^g H_m$ calculated from equations presented by all of the above authors are in good mutual agreement and also in agreement with IUPAC recommendation at 298.15 K (see Figure 4). The shape of the $\Delta_s^g C_{p,m}^0$ curve is, however, in most cases unrealistic (see Figure 5). This is not surprising because of the limited temperature ranges of the above-mentioned studies. We may conclude that the measurement error of most static measurements as quoted by authors is somewhat optimistic.

Finally, vapor pressure data obtained in this work were compared with the preliminary fit. Agreement was very good, in all cases better than 0.1 Pa. Below 273 K (i.e., for pressures below 0.8 Pa), our results tend to be lower than those from the preliminary fit (but still within the pressure difference of 0.01 Pa). Inclusion of these values in the single-property fit (without $\Delta_s^g C_{p,m}^0$ and $\Delta_s^g H_m$) would yield unrealistic $\Delta_s^g H_m$ exhibiting a maximum at a temperature of about 250 K.

Data of this work, data by van Ekeren et al.,[77] and data by Guetachew et al.,[53] which are in very good agreement with the preliminary fit, were included in the final fit (see Table 4).

Gas Saturation Method. Common problems encountered when using gas-saturation methods are incomplete saturation (in recent works this problem is usually avoided) and adsorption of material on internal walls of the apparatus. Systematic errors caused by sample impurity can be avoided in some modifications of this method.

Table 4. Data Sets on Vapor Pressure Included in the Final Fit

reference	N[a]	$T_{\min}$/K[b]	$T_{\max}$/K[c]	d/Pa[d]	$100d_r$/%[e]
Bradley and Cleasby[103]	11	279.8	293.8	0.00	1.14
Sinke[3]	1	275.0		0.90	1.00
Macknick and Prausnitz[90]	6	280.3	305.0	0.20	2.02
Colomina et al.[105]	8	271.5	284.6	0.00	1.72
van Ekeren et al.[77]	10	244.2	255.9	0.00	2.03
Sakoguchi et al.[83]	3	323.1	343.2	2.10	1.13
Guetachew et al.[53]	14	263.6	353.1	0.50	1.70
this work	55	273.5	313.5	0.00	0.85

[a] Number of experimental data points. [b] Lower temperature range of experimental data. [c] Upper temperature range of experimental data. [d] Absolute deviation, $d(p_{\mathrm{sat}}) = (\sum_{i=1}^{m_x}[p_{\mathrm{sat}}^{\mathrm{exp}} - p_{\mathrm{sat}}^{\mathrm{calc}}]_i^2/m_x)^{1/2}$. [e] Relative deviation, $d_r(p_{\mathrm{sat}}) = (\sum_{i=1}^{m_x}[(p_{\mathrm{sat}}^{\mathrm{exp}} - p_{\mathrm{sat}}^{\mathrm{calc}})/p_{\mathrm{sat}}^{\mathrm{exp}}]_i^2/m_x)^{1/2}$.

Sample removed by carrier gas was either weighed,[78-83] adsorbed and then thermally desorbed and analyzed by gas chromatography,[84] trapped in a cold trap and then analyzed by gas chromatography,[85,86] trapped in a chromatographic column and then analyzed by gas chromatography[87,88] [Clark et al.[88] used a saturation method coupled with gas chromatograph but reported only $\Delta_s^g H_m$ as (74.35 ± 1.70) kJ·mol^{-1} for temperature range (303 to 329) K which is too high.], analyzed by high-pressure liquid chromatography,[89] or combusted over a catalyst and the amount of resulting CO_2 determined.[3,90] Data are typically reported in temperature ranges of about 20 K and fitted by the simplest two parameter eq 4.

Sinke[3] and Macknick and Prausnitz[90] tried to avoid the problem of adsorption by using oxygen as a carrier gas and combusting the gaseous mixture after the saturator; in this case the sample must be very pure as burnt impurities cannot be distinguished from the burnt sample. There is no problem with impurities when analysis is done by chromatography.

Results from the above papers (with the exception of papers where data differ by more than 10 %) are compared with the preliminary fit in Figure 6, and sublimation enthalpies calculated from these data are shown in Figure 7. Overall scatter of the data is rather large. Only data by Sinke[3], Macknick and Prausnitz,[90] and Sakogushi et al.[83] are in reasonable agreement with the preliminary fit and were selected for the final fit (see Table 4).

Effusion Method. Most data measured by effusion methods were obtained from the mass of sample loss. Only de Kruif and van Ginkel[91] used a combined weighing and torsion-effusion method (data were published again by de Kruif[92]). Results of effusion method can be impaired by uncertainty in orifice area, temperature control,[93] and impurities of the measured compound. Unfortunately, most of results for naphthalene[2,91,94-100] was published only in the form of parameters of eq 4 and thus cannot be used for further smoothing. [Glukhova et al.[99,100] did not reported vapor pressures, only $\Delta_s^g H_m$ equal to 72.3 kJ·mol^{-1} in the temperature range (300 to 330) K, in reasonable agreement with preliminary fit.] A single value published by Lenoir and co-workers[101,102] was obtained by extrapolation and was not considered.

Four papers contain experimental values.[56,103-105] The data of Bradley and Cleasby[103] and Colomina et al.[105] are in good agreement with the preliminary fit (see Figure 8). Comparison of calculated enthalpies of sublimation with the preliminary fit (Figure 9), however, shows that $\Delta_s^g H_m$ calculated from vapor pressures by Colomina et al.[105] disagree with the preliminary fit; these data set will be included in the final fit with a lower weight.

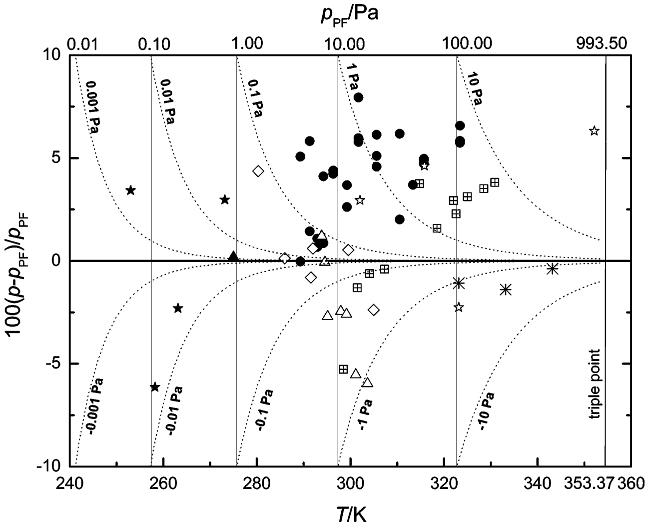

Figure 6. Gas saturation method. Deviation plot of vapor pressure data. p_{PF} is calculated from the Cox eq 9 with parameters obtained from the preliminary fit (see Table 2). ●, Gil'denblat;[79] ▲, Sinke[3]; ◇, Macknick and Prausnitz;[90] ☆, Grayson and Fosbraey;[85] △, Mironov and Khudyakov;[87] ⊞, Sato et al.;[82] ∗, Sakoguchi et al.;[83] ★, Wania et al.[84] ···, Absolute errors (0.001 Pa, 0.01 Pa, 0.1 Pa, 1 Pa, 10 Pa). Partially displayed: Grayson and Fosbraey[85] and Wania et al.[84]

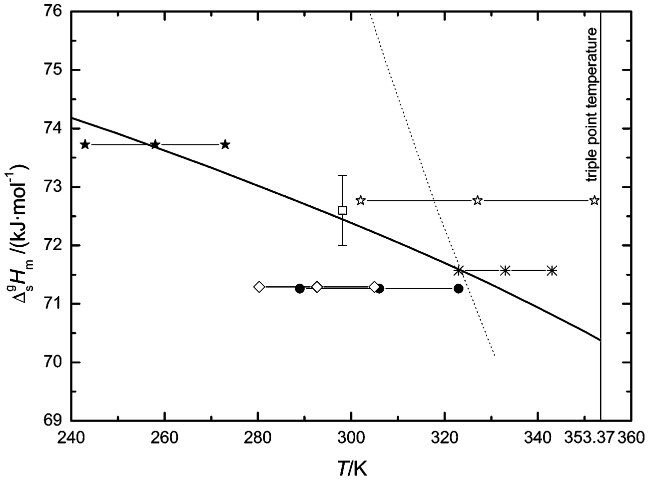

Figure 7. Gas saturation method. Comparison of $\Delta_s^g H_m$ calculated from the vapor pressure equations given by respective authors and from the preliminary fit. —, Preliminary fit; ●, Gil'denblat;[79] ◇, Macknick and Prausnitz;[90] ☆, Grayson and Fosbraey;[85] ···, Sato et al.;[82] ∗, Sakoguchi et al.;[83] ★, Wania et al.;[84] □, Sabbah et al.[5] (T = 298.15 K). Not displayed: Mironov and Khudyakov.[87]

Other Methods. This part deals with all the other methods used for measurements of vapor pressure of solid naphthalene.

Aihara[106] used a viscosity gauge to measure vapor pressures in the temperature range from (276 to 283) K. The apparatus was calibrated by measuring the vapor pressure of benzophenone. When compared with results of the preliminary fit, values of vapor pressure are from (13 to 19) % lower, and $\Delta_s^g H_m$ is lower by about 10 %.

McEachern and Sandoval[107] used a free evaporation method but reported experimental difficulties (self-cooling caused by rapid evaporation) in the case of naphthalene. Their vapor pressures as well as enthalpy of vaporization are very low compared to the preliminary fit.

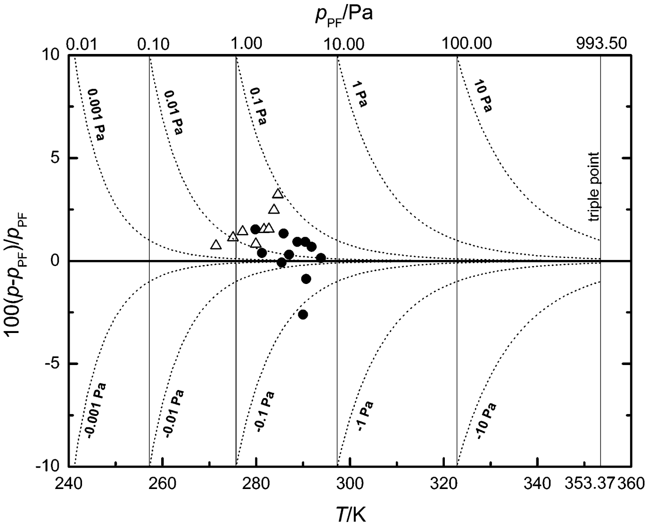

Figure 8. Effusion method. Deviation plot of vapor pressure data. p_{PF} is calculated from the Cox eq 9 with parameters obtained from the preliminary fit (see Table 2). ●, Bradley and Cleasby;[103] △, Colomina et al.[105] ···, Absolute errors (0.001 Pa, 0.01 Pa, 0.1 Pa, 1 Pa, 10 Pa). Not displayed: Radchenko and Kitaigorodskii[104] and Boller and Wiedemann.[56]

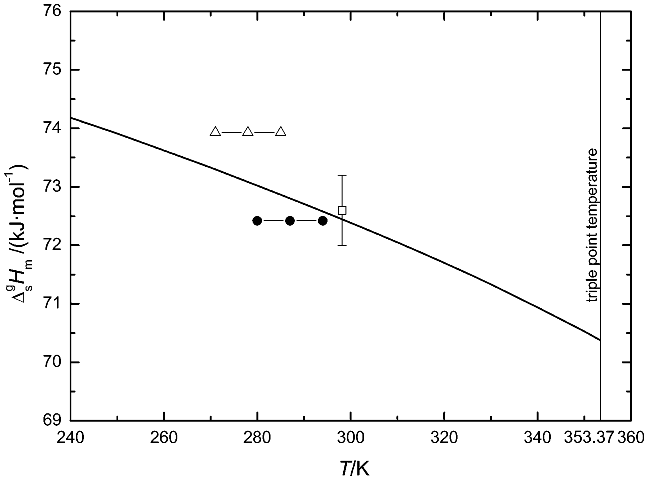

Figure 9. Effusion method. Comparison of $\Delta_s^g H_m$ calculated from the vapor pressure equations given by respective authors and from the preliminary fit. —, Preliminary fit; ●, Bradley and Cleasby;[103] △, Colomina et al.;[105] □, Sabbah et al.[5] (T = 298.15 K). Not displayed: Radchenko and Kitaigorodskii.[104]

Chickos[108] used a headspace analysis method and published smoothed data in the temperature range from (263 to 293) K. Values calculated from his equation (parameters were published by Delle Site[73]) are 2 % lower at the highest temperature and 30 % lower at the lowest temperature. The calculated $\Delta_s^g H_m$ value is about 10 % below the preliminary fit value.

All remaining values cited in this part were obtained by gas chromatography. Gas chromatography is usually used in a comparative mode (i.e., measured values are compared with those obtained with a reference compound). Vapor pressures of the reference compounds are, however, in most cases less well established than the vapor pressure of naphthalene, and resulting values cannot be therefore used for developing recommended data for naphthalene.

Moreover, the vapor pressure of a subcooled compound is usually reported. Conversion to a sublimation pressure can be done when all information needed is available (heat capacities of perfect gas and of solid, enthalpy of fusion). Even though for naphthalene all these data are available, for most other compounds these values are unavailable, and some approximations must be used. Therefore, vapor pressure measurement by a chromatographic method have large uncertainties. There are also some other simplifications commonly used with this method, discussed by Koutek et al.[109] and by Letcher and Naicker,[110] which give rise to additional uncertainties.

Bidleman[111] used eicosane (gas saturation vapor pressure data by Macknick and Prausnitz[90]) as a reference compound. Measurements were made in the temperature range from 313 K to 353 K. The only published values are two data points at 298.15 K: 22.7 Pa and 28.2 Pa for BP-1 and Apolane-87 columns, respectively. These values were converted to subcooled vapor pressures and consequently to sublimation pressures of 6.45 Pa and 8.04 Pa (conversion was done by Delle Site[73]), well below the value of 10.9 Pa obtained in the preliminary fit. Measurements were repeated by Bidleman and co-workers[112] with practically the same result of 22.65 Pa at 298.15 K.

Chickos et al.[66] used gas chromatography to determine an enthalpy of vaporization at 298.15 K for the subcooled liquid. This value was then recalculated to an enthalpy of sublimation at 298.15 K equal to 72.6 kJ·mol^{-1}, in good agreement with value of 72.45 kJ·mol^{-1} obtained by preliminary fit. No vapor pressures were reported.

Khudyakov[113] used gas chromatography in a different way (height of peaks above the zero line was measured) and published parameters of eq 4. Both calculated vapor pressures and enthalpy of sublimation value differ significantly from the preliminary fit.

Enthalpies of Sublimation. The enthalpy of sublimation of naphthalene has been reported by a number of investigators. In this part we mention the IUPAC recommended values and all direct calorimetric measurements.

The 1974 IUPAC recommendation by Cox[6] of $\Delta_s^g H_m$ (298.15 K) = (72.5 ± 0.25) kJ·mol^{-1} was based on vapor pressure data by Miller[2] and Ambrose et al.[1] and the calorimetric data by Irving[114] and Morawetz.[115] The 1987 IUPAC recommendation by Sabbah et al.[116] of $\Delta_s^g H_m$ (298.15 K) = (72.6 ± 0.3) kJ·mol^{-1} was based on the 1974 recommendation and additional vapor pressures by Colomina et al.,[105] de Kruif et al.,[9,92] and van Ekeren et al.[77] and on calorimetric data by Murata et al.[117] The 1999 IUPAC recommendation by Sabbah et al.[5] retains the 1987 IUPAC value.

Enthalpies of sublimation were recently reviewed by Chickos and Acree,[75] who selected $\Delta_s^g H_m$(298.15 K) = (72.6 ± 0.3) kJ·mol^{-1}. Besides papers cited in ref 75, five additional sources of calorimetric $\Delta_s^g H_m$ were found.[62,63,118–120] The enthalpy of sublimation has been calorimetrically measured by the carrier-gas method,[114,119] by evaporation into vacuum using an adiabatic calorimeter,[115] by a Calvet calorimeter,[116–118] and by a differential scanning calorimeter.[62–64,120,121]

Values obtained by the carrier-gas method were obtained with a commercial LKB-8721-3 and LKB-8700 calorimeters and are higher than values obtained by evaporation to vacuum. Majer and Svoboda[122] stated that the carrier-gas method is suitable for measurement of enthalpies of vaporization in the vapor pressure range from 50 Pa to 25 kPa and that evaporation techniques were developed “after the carrier gas method has been found to fail with substances exerting at 298.15 K saturated vapor pressure below 10 Pa”. Vapor pressure of naphthalene is about 10 Pa at 298.15 K; therefore, the carrier-gas method values might be dubious.

Table 5. Data Sets on Enthalpy of Sublimation Included in the Final Fit

reference	N[a]	T_{min}[b] / K	T_{max}[c] / K	d[d] / kJ·mol^{-1}	$100d_{\mathrm{r}}$[e] / %
Morawetz[115]	1	298.15		0.39	0.54
Irving[114]	1	298.15		0.56	0.77
Murata et al.[117]	22	296.00	341.10	0.34	0.47

[a] Number of experimental data points. [b] Lower temperature range of experimental data. [c] Upper temperature range of experimental data. [d] Absolute deviation, $d(\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}) = (\sum_{i=1}^{m_{\mathrm{x}}}[\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}^{\mathrm{exp}} - \Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}^{\mathrm{calc}}]_i^2/m_x)^{1/2}$. [e] Relative deviation, $d_{\mathrm{r}}(\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}) = (\sum_{i=1}^{m_{\mathrm{x}}}[(\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}^{\mathrm{exp}} - \Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}^{\mathrm{calc}})/\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}^{\mathrm{exp}}]_i^2/m_x)^{1/2}$.

On the other hand, evaporation into vacuum is a nonequilibrium process, and results should be corrected for that. Morawetz[115] added correction of 0.9 kJ·mol^{-1} to his value; Murata et al.[117] claimed that evaporation was almost at the equilibrium ("since the effusion was very slow" and "no correction was apparently needed"). Sabbah et al.[116] determined the enthalpy of sublimation using different effusion holes and claimed the smaller the orifice the better the equilibria; their values obtained with the smallest orifice are however lower than those obtained with bigger holes (and are even lower than $\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}$at the triple point). Kiselev et al.[118] used free evaporation (glass ampule broken within DAK-1−1 calorimeter) but did not mention any correction.

With the exception of $\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}$ by Torres-Gomez et al.[121] and by Rojas-Aguilar et al.,[120] values obtained by DSC are of low quality (Murray et al.[63] and Holdiness[64] even reported $\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}$without any temperature or temperature range mentioned, presumabely their values are at T_{fus}, because $\Delta_{\mathrm{s}}{}^{\mathrm{l}}H_{\mathrm{m}}$ and $\Delta_{l}^{\mathrm{g}} H_{\mathrm{m}}$were also reported) and will not be discussed.

Data by Murata et al.[117] measured above 298.15 K agree within 1 % with the preliminary fit, agreement at 298.15 K is even better. Results obtained by Torres-Gomez et al.[121] are lower than the preliminary fit by 1 %. Torres-Gomez et al.[121] also published an enthalpy of sublimation at 298.15 K. Conversion to 298.15 K using $\Delta_{\mathrm{s}}^{\mathrm{g}} C_{p,\mathrm{m}}^{0} = (-59 \pm 5)$ J·K^{-1}·mol^{-1} (taken from de Kruif et al.[9]) gave a value of $\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}} = (72.32 \pm 0.4)$ kJ·mol^{-1}, which is close to that derived from the preliminary fit. This value was not considered as it is not a direct experimental value.

When compared with values derived from the preliminary fit, data at 298.15 reported by Irving[114] and Morawetz[115] are within 0.6 % higher and 0.7 % lower, respectively. The value by Yan et al.[119] is 1.1 % higher, and the value by Kiselev et al.[118] is 1.7 % higher. Scatter of the remaining two data sets is considerable, values recommended by Sabbah et al.[116] are lower by 2.7 %, and those by Rojas-Aguilar et al.[120] are lower by 1 %. Results by Irving,[114] Morawetz,[115]and Murata et al.[117] were selected for the final fit (see Table 5).

Recommendations

This Work. Data sets of vapor pressure of solid naphthalene selected for the final fit in the preceding chapter were combined with vapor pressure and enthalpy of sublimation at the triple point and with heat capacity difference in the temperature range from 150 K to 310 K (i.e., in the same range as for the preliminary fit). The Cox eq 9 with three and four parameters was used for simultaneous correlation of the above-mentioned selected data. We found that the fourth parameter would improve fit of heat capacity difference, but calculated vapor pressures and enthalpies of vaporization remained practically unchanged. The three parameter Cox equation was selected for generating the recommended data.

Table 6. Parameters of the Cox Equation 9 from the Final Fit

A_0	A_1	A_2	T^0 / K	p^0 / Pa
3.272310	$-2.663498 \cdot 10^{-4}$	$-2.929123 \cdot 10^{-9}$	353.37	993.5

Table 7. Recommended Vapor Pressures, Enthalpies of Sublimation, and Heat Capacity Differences[a]

T / K	p / Pa	$\Delta_{\mathrm{s}}^{\mathrm{g}} H_{\mathrm{m}}$ / kJ·mol^{-1}	$\Delta H'$ / kJ·mol^{-1}	$\Delta_{\mathrm{s}}^{\mathrm{g}} C_{p,\mathrm{m}}^{0}$ / J·K^{-1}·mol^{-1}	$\Delta C'$ / J·K^{-1}·mol^{-1}
150	$1.20 \cdot 10^{-12}$	76.16	76.16	−17.31	−17.31
160	$5.42 \cdot 10^{-11}$	75.98	75.98	−18.40	−18.40
170	$1.55 \cdot 10^{-9}$	75.79	75.79	−19.48	−19.48
180	$3.04 \cdot 10^{-8}$	75.59	75.59	−20.55	−20.55
190	$4.33 \cdot 10^{-7}$	75.38	75.38	−21.61	−21.61
200	$4.69 \cdot 10^{-6}$	75.16	75.16	−22.66	−22.66
210	$4.02 \cdot 10^{-5}$	74.93	74.93	−23.71	−23.71
220	$2.82 \cdot 10^{-4}$	74.69	74.69	−24.75	−24.75
230	$1.66 \cdot 10^{-3}$	74.43	74.43	−25.78	−25.78
240	$8.37 \cdot 10^{-3}$	74.17	74.17	−26.80	−26.80
250	$3.69 \cdot 10^{-2}$	73.90	73.90	−27.82	−27.81
260	0.1446	73.62	73.62	−28.83	−28.82
270	0.509	73.32	73.32	−29.85	−29.82
280	1.63	73.02	73.02	−30.87	−30.81
290	4.798	72.70	72.71	−31.92	−31.79
298.15	10.92	72.44	72.44	−32.81	−32.59
300	13.08	72.38	72.38	−33.02	−32.77
310	33.28	72.04	72.05	−34.21	−33.74
320	79.56	71.69	71.71	−35.56	−34.70
330	179.7	71.32	71.36	−37.15	−35.65
340	385.4	70.94	71.00	−39.11	−36.59
350	788.4	70.52	70.63	−41.61	−37.53
353.37	993.5	70.38	70.50	−42.62	−37.85

[a] $\Delta H'$and $\Delta C'$ are defined by eqs 2 and 3.

Results of the fit are presented in Tables 6 and 7. It should be noted that results of the final fit are practically identical with the preliminary fit. This indicates good consistency of vapor pressures selected for the final fit with other thermodynamically related properties. Agreement in the low-pressure region (below 1 Pa, i.e., below 275 K) is not surprising because in this temperature range heat capacities were assigned higher weight in comparison with vapor pressures. A similar approach was used by Wagner et al.[123] in their work on recommended sublimation pressures of ice.

Comparison with Previous Recommendations. All previous recommendations for the enthalpy of sublimation at 298.15 K are in mutual agreement and in agreement with the recommended value from this work. Recommendations for vapor pressure of solid naphthalene were made by Sinke[3], Ambrose et al.[1], de Kruif et al.,[9] Chirico et al.,[7] van den Linde et al.,[47] and van Genderen and Oonk.[61]

Sinke[3] combined his single experimental data point with selected literature data and ensured consistency of selected data sets with vibrational assignment/spectroscopic data. He published a table of nine values in the temperature range from 220 K to the triple point. Ambrose et al.[1] used only their own data in development of recommended values. De Kruif et al.[9] used only data measured in their laboratory and found a good agreement with Ambrose's data. The same data were used also by van Genderen and Oonk.[61] Chirico et al.[7] disregarded all previous data and used a "third-law" method to calculate sublimation pressures. Van den Linde et al.[47] found none of the published

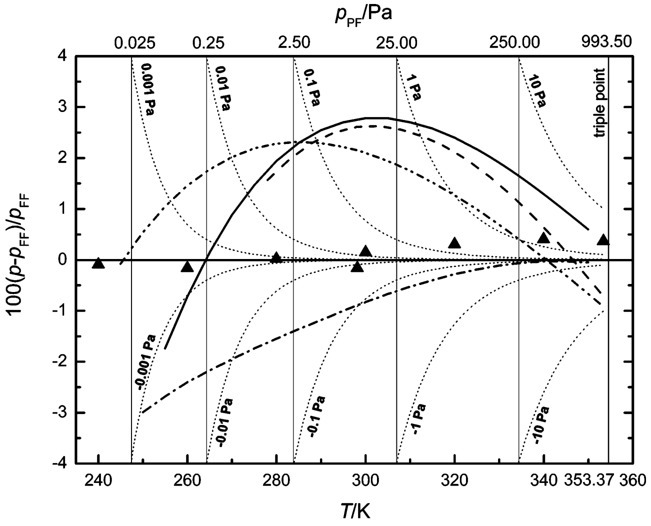

Figure 10. Comparison of vapor pressure obtained from the final fit with previous recommendations. ▲, Sinke[3]; —, Ambrose et al.;[1] – –, de Kruif et al.;[9] ·-·-·, Chirico et al.;[7] -··, van der Linde et al.[47] ···, Absolute errors (0.001 Pa, 0.01 Pa, 0.1 Pa, 1 Pa, 10 Pa).

data sets whose "individual precisions and mutual consistency would dominate the others" and used all existing data to produce recommended values.

All the above-mentioned recommendations are graphically shown in Figure 10. Recommendation by Sinke[3] is in excellent agreement with our recommendation, differences being smaller than 0.5 % in all cases. Recommended vapor pressures by Chirico et al.[7] are always lower than our recommended values, differences are however small in both absolute and relative values.

Remaining recommendations[1,9,47,61] intersect our values, but agreement is only moderate. Enthalpy of sublimation at the triple point calculated from these recommendations would be lower than our recommended value derived from the vapor pressure data by 0.5 kJ·mol^{-1} (Ambrose et al.[1]) or by 1 kJ·mol^{-1} (remaining recommendations). At low temperatures, calculated $\Delta_s^g H_m$ would be higher than our recommended data.

A comparison of the enthalpy of sublimation derived from the final fit with selected calorimetric values and with $\Delta_s^g H_m$derived from previous recommendations is shown in Figure 11.

Figure 12 compares $\Delta_s^g C_{p,m}^0$ derived from the final fit and derived from previous recommendations. Only $\Delta_s^g C_{p,m}^0$ derived from the final fit agrees well with that obtained from experimental solid heat capacities by Chirico et al.[8] and from perfect gas heat capacities by Frenkel et al.[72] The recommended data by Chirico et al.[7] start to deviate below about 280 K. All remaining recommendations (Ambrose et al.,[1] de Kruif et al.,[9] van den Linde et al.[47]) lead to an erroneous temperature dependence of $\Delta_s^g C_{p,m}^0$.

Conclusion

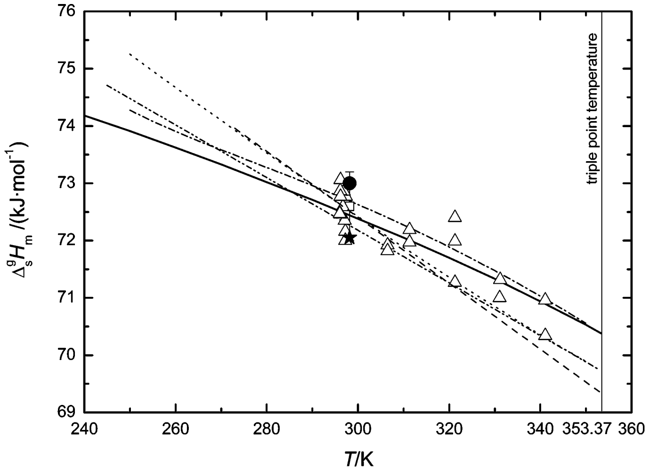

Figure 11. Comparison of $\Delta_s^g H_m$ derived from the final fit with selected direct calorimetric values and with $\Delta_s^g H_m$ derived from previous recommendations. —, final fit; ···, Ambrose et al.;[1] – –, de Kruif et al.;[9] ·-·-·, Chirico et al.;[7] -··, van der Linde et al.;[47] ★, Morawetz;[115]; ●, Irving;[114] △, Murata et al.;[117] □, Sabbah et al.[5] (T = 298.15 K).

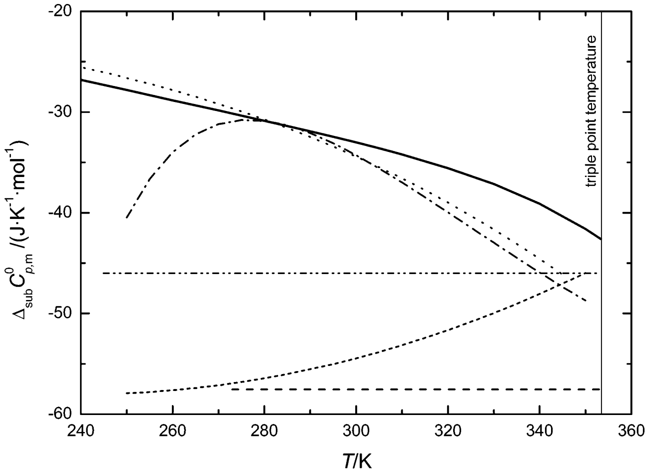

Figure 12. Comparison of $\Delta_s^g C_{p,m}^0$ derived from the final fit and from previous recommendations. —, final fit; ···, $C_{p,m}^{g0}$ from Frenkel et al.[72] and $C_{p,m}{}^s$ taken from Chirico et al.;[8] - - -, Ambrose et al.;[1] – –, de Kruif et al.;[9] ·-·-·, Chirico et al.;[7] -···, van der Linde et al.[47]

Recommended vapor pressure and enthalpy of sublimation in the temperature range from 150 K to the triple point temperature, 353.37 K, of solid naphthalene was developed by a multi-property fit of selected experimental vapor pressure data measured by the static method, by the gas saturation method, and by the effusion method and of the related thermal data, selected calorimetrically measured enthalpies of sublimation and differences in solid and perfect gas heat capacities. Experimental vapor pressure and experimental enthalpy of sublimation data was selected by comparing the literature data with a preliminary recommendation obtained from a simultaneous correlation of vapor pressure at the triple point, enthalpy of vaporization and enthalpy of fusion at the triple point and differences in solid and perfect gas heat capacities. Recommended data of solid naphthalene, vapor pressure, and enthalpy of sublimation are consistent with well-established literature values for liquid naphthalene and also with the selected thermal data for the solid−vapor equilibrium.

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