Vapor Pressure of Organic Compounds. Measurement and Correlation

Květoslav Růžička[1], Michal Fulem[1,2], Vlastimil Růžička[1]

[1] *Department of Physical Chemistry, Institute of Chemical Technology, 166 28 Prague 6, Czech Republic* (kvetoslav.ruzicka@vscht.cz, vlastimil.ruzicka@vscht.cz)

[2] *Institute of Physics, Academy of Sciences of the Czech Republic, 162 00 Prague 6, Czech Republic* (michal.fulem@vscht.cz)

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1. Introduction

The vapor-liquid saturation line in a diagram of pressure versus temperature is the main characteristic of the vaporization equilibrium for a one-component system. The vapor pressure

p_{sat} is one of the most frequently measured thermodynamic properties for pure organic liquids, and the normal boiling temperature T_b is a basic physicochemical parameter for any substance. Vapor pressure data p_{sat} are needed for a variety of chemical engineering and thermodynamic calculations. Importance of vapor pressure data, in particular for high-boiling organic compounds, became even more evident over the last several decades with raising awareness of the environmental impact of pollutants.

The experimental determination of vapor pressure is relatively easy in the range between 1 and 200 kPa which is usually denoted as a moderate (or medium) pressure region. Most published data have been reported between 5 and 100 kPa and many reliable results are available. The best accuracy can be achieved near the normal boiling temperature; the high quality data measured close to atmospheric pressure have an error below 0.01 percent. Several compilations were published over the last 30 years (see Appendix A) that present experimental and/or recommended data for a large quantity of compounds.

Measurements become difficult at low pressures (say $p_{sat} < 1$ kPa); data are available only for a limited number of substances and often subject to large systematic errors. Differences in reported values usually amount to several tens of percent near the triple point temperature. Various approaches to experimental determination of vapor pressures were reviewed (see Appendix B). The main experimental techniques for determination of vapor pressures in the low-pressure region are the saturation method using a carrier gas and two techniques based on molecular effusion (weighing effusion and torsion effusion methods). Gas-liquid chromatography has also been used, but it is not easy to give the resulting data a rigorous thermodynamic interpretation. Direct static measurement of vapor pressure is a universal technique that can be used over a wide pressure range down to, or in special cases even below, 1 Pa; the most accurate data reported in the low-pressure region were obtained by this technique.

2. Measurement of Vapor Pressure by a Static Method

In our laboratory two static apparatuses are currently available. Another static apparatus especially suited for measurements with highly toxic compounds was constructed in a partner laboratory of an institute of the Academy of Sciences of the Czech Republic[30]. Static method allows measurement of vapor pressure in the liquid as well in the solid phases over a wide range of temperatures including room temperature. As the inner volume of the apparatuses is evacuated to pressure of about 10^{-5} Pa and the apparatus is regularly checked for tightness by a helium leak detector the static apparatuses allow measurement with compounds sensitive to oxygen and water. In the next two sections the apparatuses and their most recent improvements are described in some more details and the preparation of samples for vapor pressure measurement is discussed.

Apparatus for the vapor pressure measurement

Two static apparatuses internally denoted as STAT3 and STAT4 (see Fig. 1 and Fig. 2, respectively) were recently built in our laboratory at the Institute of Chemical Technology, Prague. Working ranges of apparatuses STAT3 and STAT4 are given in Table 1.

Apparatus	Pressure range	Temperature range	Accuracy in pressure	Accuracy in temperature
STAT3	0.1 Pa to 13 kPa	40 to 200 °C	0.2 % (0.1-13 kPa) 1 % (10-100 Pa) 3 % (1-10 Pa) 10 % (0.1-1 Pa)	0.02 °C
STAT4	0.1 Pa to 1.3 kPa	-40 to 40 °C	0.05% or $\sigma(p/\mathrm{Pa}) = 0.005(p/\mathrm{Pa}) + 0.05$	0.02 °C

Both apparatuses are constructed of 1/4” stainless steel internally electrochemically polished tubing with VCR fittings and NUPRO valves (Swagelok Co., USA). Valves taking control of measuring procedure are computer controlled using HP-VEE program and servo PPN2 (Ekorex, Czech Republic). Pressure is measured by capacitance diaphragm MKS pressure gauges (MKS Baratron™ 616A11TRC-S and MKS Baratron™ 690A11TRA, respectively, MKS Instruments Inc., USA) and sample temperature is measured by the platinum resistance thermometers Burns Engineering 12001-A-12-6-2-A (Burns Engineering Inc., USA) in a four-wire connection. The thermometers Burns Engineering are calibrated at the ice point and/or by comparison to standard platinum resistance thermometer (SPRT). This SPRT is calibrated to the ITS-90 and its calibration is traceable to the National Institute of Standards and Technology (NIST). The accuracy of the measurement of sample temperature is very important and is estimated to be better than 0.02 K. In the case of STAT3 the sample temperature is controlled by metal thermostat built in our laboratory and in the case of STAT4 by liquid thermostat Lauda RK 8 CP (Lauda, Germany). Stability of the sample temperature is within 0.02 K in both cases.

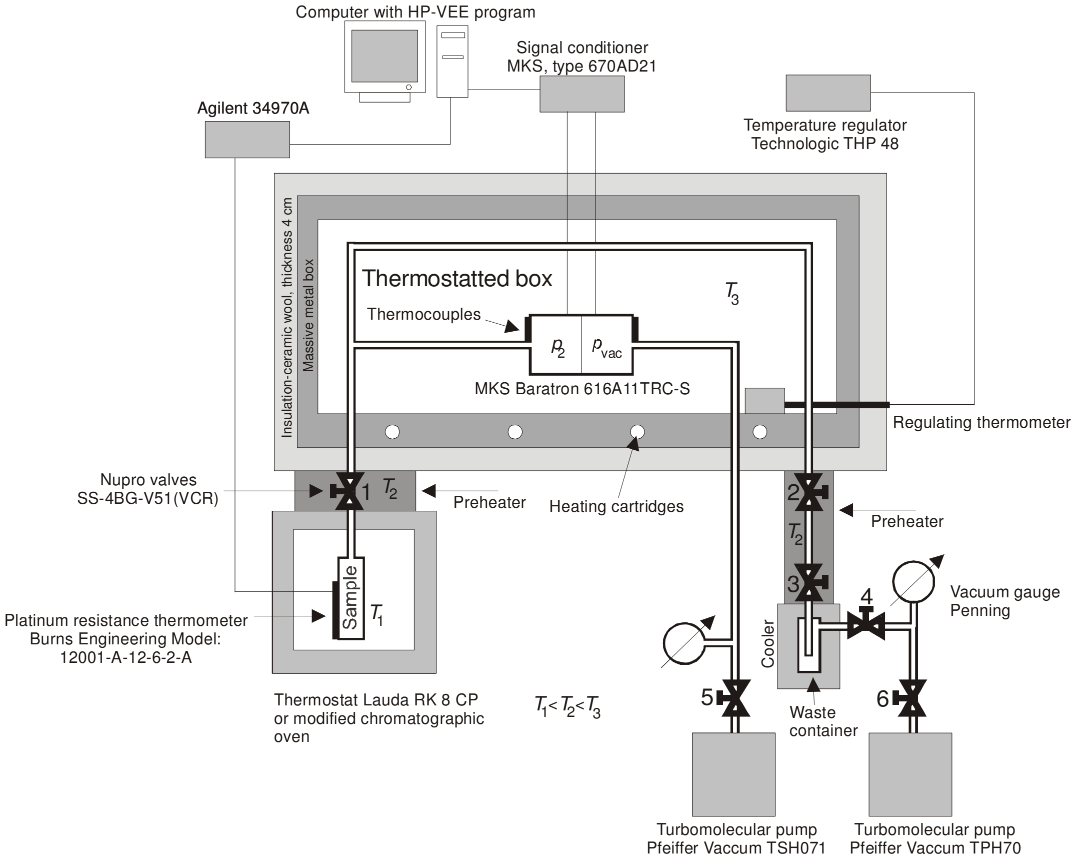

Fig. 1 Apparatus STAT3 for the measurement of vapor pressure. Valve 1 is the container valve; valves 2 and 3 are computer controlled. Valves 3-6 serve for the maintenance of the apparatus.

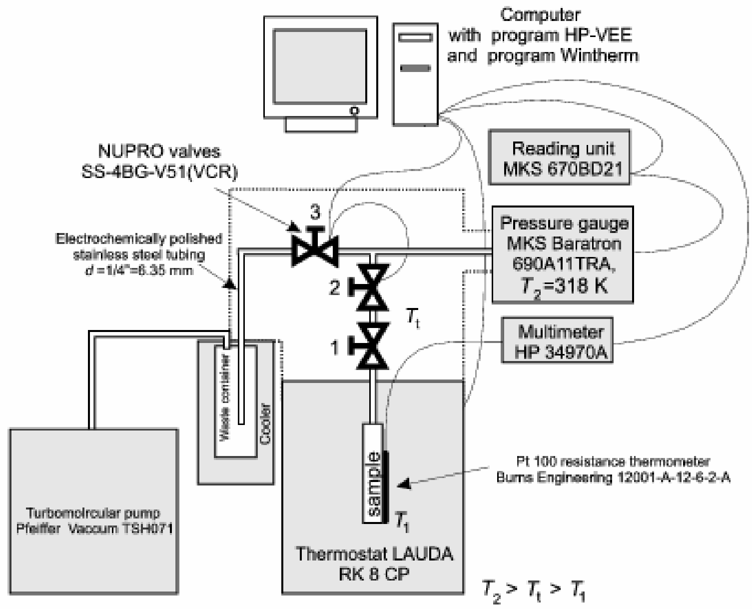

Fig. 2 Apparatus STAT4 for the measurement of vapor pressure. Valve 1 is the container valve; valves 2 and 3 are computer controlled.

Prior to measurement of vapor pressure the apparatuses are checked for tightness by MKS PICO™ vacuum leak detector (MKS Instruments Inc., USA). The apparatuses are evacuated between individual measurement cycles by turbomolecular pumps to a pressure of 10^{-5} Pa. A computer using HP-VEE program monitors the pressure, the temperature of the sample, preheater and thermostatted box (see Fig. 1) and controls the measuring procedure. Experiments are carried out in the given temperature interval by varying the temperature at random in order to avoid systematic errors caused by possible decomposition or insufficient degassing of the sample.

Preparation of samples prior to vapor pressure measurement

Generally, there are two steps in preparation of samples for vapor pressure measurement by a static method. Firstly, since vapor pressure is very sensitive to sample impurities it is often necessary to purify and dry the sample. Secondly, the samples must be perfectly degassed. This step is a prerequisite for correct vapor pressure measurement by a static method. Several methods of degassing are known: the method based on repeated freeze-pump-melt cycles,[4] degassing using ultrasound, distillation, etc. We developed a new method, which allows handling of compounds without any risk of contamination and loss of the sample during degassing procedure. The method is based on using a semi permeable membrane (e.g. made of polydimethylsiloxane) which is permeable only for low molecular weight gases (oxygen, nitrogen, etc.) but not for the sample molecules. This membrane is placed between the sample cell and the vacuum pump to avoid loss of the sample when it is pumped out by a vacuum pump; pressure is maintained at or below 1 Pa. This method proved to be very efficient and easy when using a simple vacuum apparatus.

3. Simple and Controlled Extrapolation of Vapor Pressures towards the Triple Point

The simplest approach to obtain vapor pressure data in the low-pressure region is an extrapolation from vapor pressures measured in the medium pressure region using an equation with an optimum number of parameters. The input data must be reliable and available over a sufficiently wide temperature interval in order to allow a meaningful extrapolation. The form of the correlation equation used can also largely affect the results.

An alternative approach regarding extrapolation towards low pressures is a combination of p_{sat} in the medium pressure region with the related thermal data by which we understand enthalpy of vaporization ΔH_{vap} and the heat capacity difference $\Delta C^0_{\mathrm{vap}}$. The latter quantity is defined as

$$\Delta C^0_{\mathrm{vap}} = C_p^{g0} - C_p^{\ell} \tag{1}$$

where C_p^{g0} denotes the heat capacity of an ideal gas and C_p^{ℓ} that of the liquid. Vapor pressures are related to the thermal properties by the exact thermodynamic relationships, which allow a controlled extrapolation of p_{sat} data in the medium-pressure region down to the triple-point temperature T_{t}, provided the thermal data are available in the temperature range below that of the p_{sat} data. In extrapolations, enthalpies of vaporization cannot always be used effectively, as reliable calorimetric values at temperatures corresponding to p_{sat} in the low-pressure region are available only for a limited number of compounds. On the other hand, heat capacity differences are more readily accessible since they can be calculated for many compounds in a wide temperature range down to the triple-point temperature by combining calorimetric and spectroscopic data. The simultaneous correlation of medium vapor pressures and $\Delta C^0_{\mathrm{vap}}$ values can also be useful for determining the frequently required values of ΔH_{vap} at 298.15 K for high boiling compounds. Further combination of the vapor pressure calculated at T_{t} with the enthalpies of phase transition (solid-liquid, solid-solid) and differences between the heat capacity of an ideal gas and that of the solid makes it possible to calculate vapor pressures along the vapor-solid saturation line.

The method using the thermal data for extrapolating vapor pressures was first described by King and Al-Najjar[3], and further developed by Ambrose and Davies[5] and Růžička and Majer.[7] Thermodynamic background of the method of multi-property simultaneous correlation of vapor pressure and related thermal data is described in the part 3.

Růžička and Majer[12] tested several most frequently used equations for correlating temperature dependence of vapor pressure. The Antoine equation

$$\ln p_{\mathrm{sat}} = A_1 - \frac{A_2}{T + A_3} \tag{2}$$

clearly shows the poorest performance; it fails for most types of compounds both in simple and controlled extrapolation and is not even able to describe adequately the p_{sat} data in the medium-pressure region for compounds with specific interactions. The Antoine equation has a very low flexibility and its use should always be abandoned when the temperature interval of correlation becomes large (say above 50 K) and any kind of extrapolation is foreseen. The only effective way of using the Antoine equation is determination of two (or more) parameter sets, corresponding to different temperature intervals, with forced continuity of p_{sat} and its first temperature derivative at the boundaries (TRC Thermodynamic Tables[20, 21]).

The Wagner equation[2]

$$\ln\left(\frac{p_{\mathrm{sat}}}{p_{\mathrm{c}}}\right) = \frac{T_{\mathrm{c}}}{T}\sum_{i=1}^{m} A_i \left(1 - \frac{T}{T_{\mathrm{c}}}\right)^{\alpha_i} \tag{3}$$

requires the use of critical parameters that provide for the realistic prediction of the vapor pressure saturation line up to the critical temperature. However, this constraint limits the flexibility of the relationship in low-pressure extrapolations and is both useless and inconvenient for high boiling chemicals that decompose below or near the normal boiling temperature. The number of adjustable parameters in equation (3) is usually four; five adjustable parameters were used exceptionally for correlations of accurate data in a wide temperature range. In all versions of the Wagner equation the first exponent α_1 is equal to 0. The four-parameter forms with either $\alpha_2=1$, $\alpha_3=2$, $\alpha_4=5$ or $\alpha_2=1.5$, $\alpha_3=3$, $\alpha_4=6$ have been used most often.

The Cox equation[1]

$$\ln\left(\frac{p_{\mathrm{sat}}}{p_{\mathrm{o}}}\right) = \left(1 - \frac{T_{\mathrm{o}}}{T}\right) \exp\left(\sum_{i=0}^{n} A_i T^i\right) \tag{4}$$

can be considered to be the most useful equations for extrapolations toward low pressures; the possibility of changing both the number of parameters and the reference condition T_o and p_o allows one to obtain different forms suitable for particular applications. The three-parameter form with the normal boiling point ($T_o=T_b$ and p_o=101,325 kPa) is very dependable in both simple and controlled extrapolation for all organic liquids with the exception of hydrogen-bonded compounds. In the latter case, the four-parameter equation gives very good results for extrapolation when vapor pressures and the thermal data are fitted simultaneously. For compounds decomposing below the normal boiling temperature, a vapor pressure corresponding to a lower temperature can always be used as a reference condition. On the other hand, the use of the critical point allows one to transform the Cox equations into a relationship suitable for description of the complete vapor pressure line. The four-parameter form with reference conditions T_{c} and p_{c} is comparable to the Wagner equation and behaves similarly in correlation and extrapolation toward low pressures. The Wagner equations require the use of critical parameters that provide for the realistic prediction of the vapor-pressure saturation line up to the critical temperature. However, this constraint limits the flexibility of the relationship in low-pressure extrapolations and is both useless and inconvenient for high boiling chemicals that decompose below or near the normal boiling temperature.

4. Thermodynamic Background of the Data Correlation

Thermodynamic background for the temperature correlation of vapor pressures and the related thermal data has been described in the literature (Majer et al.[8]; Růžička and Majer[11]) and will be reviewed only briefly here. The parameters of a selected correlation equation can be determined by minimizing a general objective function:

$$S=\sum_{i=1}^{t}\frac{\left(\ln p_{\mathrm{sat}}^{\mathrm{exp}}-\ln p_{\mathrm{sat}}^{\mathrm{sm}}\right)_i^2}{\sigma_i^2\ln p_{\mathrm{sat}}}+K_H^2\sum_{j=1}^{u}\frac{\left(\Delta H'^{\,\mathrm{exp}}-\Delta H'^{\,\mathrm{sm}}\right)_j^2}{\sigma_j^2\Delta H'}+K_{\mathrm{C}}{}^2\sum_{k=1}^{v}\frac{\left(\Delta C'^{\,\mathrm{exp}}\ \Delta C'^{\,\mathrm{sm}}\right)_k^2}{\sigma_k^2\Delta C'} \qquad (5)$$

The three individual sums correspond to the contribution of vapor pressures, enthalpies of vaporization, and heat capacity differences; indices *t, u, v* indicate the number of data points for each property. In the case when $u = v = 0$, the preceding equation reduces to the common formula for the weighted least squares fitting of vapor pressures alone; K_H, K_c are the factors allowing one to modify the weight of the thermal properties in the correlation; their values differ from unity when the number of data points for individual properties is disproportional or when some data inconsistency is observed. The variances $\sigma^2\ln p_{\mathrm{sat}}$, $\sigma_i^2\Delta H'$, $\sigma_i^2\Delta C'$ are estimated from the expected errors of experimental data points

The quantities with the superscript “sm” are expressed from the selected vapor pressure equation ($p_{\mathrm{sat}}{}^{\mathrm{sm}}$); the quantities $\Delta H'^{\mathrm{sm}}$ and $\Delta C'^{\mathrm{sm}}$ are given by equations

$$\Delta H' = \mathrm{R}T^2\left(\frac{\mathrm{d}\ln p}{\mathrm{d}T}\right)_{\mathrm{sat}} \qquad (6)$$

$$\Delta C' = \left(\frac{\mathrm{d}\Delta H'}{\mathrm{d}T}\right)_{\mathrm{sat}} = R\left[\frac{\mathrm{d}}{\mathrm{d}T}\,T^2\left(\frac{\mathrm{d}\ln p}{\mathrm{d}T}\right)\right]_{\mathrm{sat}} \qquad (7)$$

The quantities with the superscript "exp" relate to experimental vapor pressures ($p_{\mathrm{sat}}{}^{\mathrm{exp}}$); and thermal data. $\Delta H'^{\mathrm{exp}}$ and $\Delta C'^{\mathrm{exp}}$ can be calculated from ΔH_{vap} and $\Delta C^{\circ}_{\mathrm{vap}}$ as follows:

$$\Delta H' = \frac{\Delta H}{1+\dfrac{p_{\mathrm{sat}}}{RT}\left(B-V^{\ell}\right)} \qquad (8)$$

$$\Delta C' = \Delta C^0_{\mathrm{vap}} - T p_{\mathrm{sat}} \frac{\mathrm{d}^2 B}{\mathrm{d}T^2} - 2T \frac{\mathrm{d}(B - V^{\ell})}{\mathrm{d}T}\left(\frac{\mathrm{d}p}{\mathrm{d}T}\right)_{\mathrm{sat}} - T(B - V^{\ell})\left(\frac{\mathrm{d}^2 p}{\mathrm{d}T^2}\right)_{\mathrm{sat}} \tag{9}$$

where B is the second virial coefficient and the pressure dependence of the molar volume V^{ℓ} is neglected. For ideal gas behavior, $\Delta H'$ and $\Delta C'$ are equal to ΔH_{vap} and $\Delta C^0_{\mathrm{vap}}$, respectively. This means that at sufficiently low pressures the primed quantities and the thermal data are practically identical and the importance of the pVT correction terms is increasing with increasing vapor pressure. At the normal boiling temperature, the quantities $\Delta H'$ and $\Delta C'$ differ from ΔH_{vap} and $\Delta C^0_{\mathrm{vap}}$ typically by about 5 and 40 %, respectively. The possibilities of accurately determining the pVT correction terms in Eqs. 8 and 9 are limited for most compounds. In order to avoid distortion of the correlation through uncertainty in estimating the vapor nonideality, it is necessary to confine thermal data to the region where correction terms are not important, that is, $T<T_b$-40 and $T<T_b$-80 for ΔH_{vap} and $\Delta C^0_{\mathrm{vap}}$, respectively.

The simultaneous treatment of vapor pressures and the related thermal data requires that reliable data are available for the respective properties. The data availability has been substantially facilitated over the last few decades by the publication of several comprehensive compilations listing the evaluated data for thermal properties in the form of correlating equations. Calorimetric enthalpies of vaporization were compiled and the recommended data produced for over 650 compounds by Majer and Svoboda [6], and experimental heat capacities of liquid were evaluated and correlated as a function of temperature for more than 2000 compounds by Zábranský et al.[13, 19] Frenkel et al. [10] evaluated ideal gas properties for over 2000 organic compounds and reported recommended values of C_p^{g0}. Bureš et al. [9] published a temperature correlation of thermodynamic properties of ideal gas (including spectroscopic C_p^{g0} values) for 3000 organic compounds.

5. Compounds Studied in Our Laboratory

Several families of compounds have been studied so far in our laboratory. The families include organic pollutants (chlorobenzenes, phthalates), high-boiling and poly-condensed compounds of petroleum interest, two compounds of pharmaceutical interest, metal-organic compounds, alkane-α,ω-diamines as biochemical model compounds, and isomeric pentanols. We also measured and developed recommended data for vapor pressure of solid naphthalene which is used as a standard compound for vapor pressure measurements. A survey of compounds measured with respective references is given in the table 1.

In several cases we have collaborated with other laboratories where complementary techniques are available. These include Institute of Physics, Academy of Sciences of the Czech

Republic (*static method for toxic substances*, Eduard HULICIUS), E. Hála Laboratory of Thermodynamics, Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic (*ebulliometry*, Karel AIM), Laboratoire d'Instrumentation et de Chimie Analytique en Solution, Université Claude Bernard, 69622 Villeurbanne, France (*static method*, Jacques JOSE, Ilham MOKBEL), Department of Chemistry, Belarusian State University, Minsk, Belarus (*Knudsen effusion method*, Dzmitry H. ZAITSAU, Gennady J. KABO), University of Porto, Faculty of Science, Department of Chemistry, Porto, Portugal (*Knudsen effusion method*, Manuel Joao S. MONTE), Laboratoire de Thermodynamique des Solutions et des Polymeres, Université Blaise Pascal, Aubière, France (*calorimetric measurements*, Vladimír MAJER), Institute of Physical Chemistry, Faculty of Chemistry and Physics, Technical University - Bergakademie Freiberg, Freiberg/Sachsen, Federal Republic of Germany (*calorimetric measurements*, H.-G. SCHMIDT, Gert WOLF), former Chemical Thermodynamics Group, Utrecht University, The Netherlands (*calorimetric measurements*, Aad van GENDEREN, J. Cees van MILTENBURG).

Table 1. **Survey of compounds studied in our lab** (vapor pressure measurement was performed in all cases)

Family	Compounds	References	Note
Chlorobenzenes	di-, tri-, penta-chlorobenzenes	Roháč et al. [16]	Correlation of own and literature data by SimCor[1], recommended data.
High-boiling and poly-condensed compounds of petroleum interest	phenanthrene, pyrene, benzo[a]pyrene, 1,2,3,4-tetrahydronaphthalene, acenaphthene, 1,2-dihydronaphthalene, dibenzothiophene, 1-phenyldodecane, (5α)-cholestane, adamantane	Růžička et al.[14], Mokbel et al. [17]	Correlation of own and literature data by SimCor, recommended data from 220 to almost 600 K.
Esters of phthalic acid	dimethyl-, diethyl-phthalate	Roháč et al. [15, 26]	Correlation of own and literature data by SimCor, recommended data
Compounds of pharmaceutical interest	perhydroacenaphthylene, perhydrophenanthrene	Roháč et al. [18]	Only vapor pressure data determined by ebulliometry.
Metal-organic compounds	diethylzinc, triethylantimony, trimethylgallium, trimethylalluminum, $Y(thd)_3$ and $Zr(thd)_4$[2], trimethylindium, di-tert-butylsilane, trimethyl phosphine, tert-butyl arsine, bis(cyclopentadienyl) manganese, tert-butyl lithium	Fulem et al. [22, 24, 25, 27, 30, 32]	Only vapor pressure data determined by static method.

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[1] SimCor = multi-property simultaneous correlation of vapor pressure and related thermal data

[2] thd=2,2,6,6-tetramethylheptane-3,5-dionate

Family	Compounds	References	Note
Metal-organic compounds	trimethylgallium and trimethylaluminium	Fulem et al. [29]	Params. of Antoine and Cox eqns. derived by SimCor from the most reliable vapor pressure data.
Calibration standards	Naphthalene	Růžička et al. [28]	Recommended solid p_{sat} consistent with calorimetric enthalpies of sublimation and with properties at the triple point derived by SimCor.
Alkane-α,ω-diamines	NH_2-$(CH_2)_n$-NH_2 ($5 \leq n \leq 8$)	Fulem et al. [23]	Params. of Cox eqn. derived by SimCor from selected p_{sat} and heat capacity differences. Enthalpies of vaporization and of sublimation calculated.
C_5 alkanols		Růžička et al. [31]	Recommended liquid p_{sat} consistent with calorimetric enthalpies of vaporization and heat capacity differences derived by SimCor.

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Symposium on Thermophysical Properties, Boulder, CO, USA, July 30 - August 4, 2006; NIST/ASME, Boulder, CO, USA: Boulder, CO, USA, 2006.

32. Pangrác, J.; Samochin, E.; Šimeček, T.; Melichar, K.; Hulicius, E.; Růžička, K.; Fulem, M.; Morávek, P.; Růžička, V.; Rushworth, S. A. In *Vapour pressure study of Mn(cp)2 and t-BuLi organometallics*, 12th European Workshop on MOVPE, Bratislava, Slovakia, June 3rd - 6th, 2007; Bratislava, Slovakia, 2007; pp 37-40.

Appendix A: Sources of vapour pressure data

Presented list of sources of vapour pressure data of is definitely not complete. Suggestions for including other sources as well as notification about errors are welcomed (ruzickak@vscht.cz).

Whenever possible, ISBN of books or www link for on-line sources is presented. Older sources which were later updated are in gray

Some other sources can be found at http://www.epa.gov/libraries/core/chem.htm and http://en.wikipedia.org/wiki/Vapor_pressure

List is divided into three sections:

- Books/databanks for technological applications (items 1 to 12)
- Books/databanks for environmental applications (items 20 to 22)
- Review papers in scientific journals (items 50 to 57)

1A) Ohe, S. Computer Aided Data Book of Vapor Pressure. 1976, Tokyo, Data Book Publishing. ISBN not found. http://s-ohe.com/VP_1ST.html
Ohe published book with datasets represented graphically (graph for each dataset includes also literature citation, and parameters of Antoine eq).
Number of compounds not specified.

1B) Ohe, S. Computer Aided Data Book of Vapor Pressure. 2nd Edition. 1999, Tokyo, Data Book Publishing 1999. [ISBN: 4-902209-04-7] 1550 pp., USD 1400 http://www.s-ohe.com/katarogu.html , www.data-books.com (in Japanese).
Second edition of book by Ohe contains 3024 datasets represented graphically (no numeric values). Graphs include also literature citation, parameters of Antoine eq, temp. and pressure range, and "error" in mmHg).
Number of compounds not specified.

2A) Boublík, T., V. Fried, and E. Hála, The Vapour Pressures of Pure Substances. Selected values of the temperature dependence of the vapour pressures of some pure substances in the normal and low pressure region. 1973, Amsterdam: Elsevier. [ISBN 0-444-41097-X] 626 pp.

2B) Boublík, T., V. Fried, and E. Hála, The Vapour Pressures of Pure Substances. Selected values of the temperature dependence of the vapour pressures of some pure substances in the normal and low pressure region. 2nd Edition, 1984, Amsterdam: Elsevier.
[ISBN 0-444-42266-8] 972 pp.
Original datapoints (recalculated to °C and kPa) are presented along with data calculated from Antoine eq and corresponding absolute and percent deviation from the fit. Antoine eq parameters and standard deviation is are also given (points with standard deviation exceeding st.dev more than three times are excluded and fitting procedure is repeated). When there are several data sets for given compounds, each dataset is treated separately.
Number of compounds/datasets not stated.
Valuable source of information for hydrocarbons (API project).

3A) Dykyj, J. and M. Repáš. Tlak nasýtenej pary organických zlúčenín (Vapor pressure of organic compounds). Volume 1 (1979) Bratislava, Veda (in Slovak). No ISBN. 516 pp

3B) Dykyj, J. Repáš. M., and Svoboda, J. Tlak nasýtenej pary organických zlúčenín (Vapor pressure of organic compounds). Volume 2 (1983) Bratislava, Veda (in Slovak). No ISBN. 427 pp
Monographs by Dykyj et al. (in Slovak) contain parameters of Antoine eq, references to both accepted and rejected literature sources, and quality reating. Though it does not contain original datapoints, it covers data for large amount of compounds extracted from several thousands of literature sources. Data for solids are also included. Volume two represents update of data for compounds included in Vol. 1 as well as data for new compounds.

3Ca) Dykyj, J., J. Svoboda, R.C. Wilhoit, M. Frenkel, and K.R. Hall, Vapor Pressure and Antoine Constants for Hydrocarbons, and S, Se, Te, and Halogen Containing Organic Compounds Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology. Vol. 20A. 1999, Heidelberg: Springer. [ISBN 978-3-540-64735-5] (data for 4252 compounds) 373 pp, price EUR 3809,
http://www.springer.com/laboe/book/978-3-540-64735-5
3Cb) Dykyj, J., J. Svoboda, R.C. Wilhoit, M. Frenkel, and K.R. Hall, Vapor Pressure and Antoine Constants for Oxygen Containing Organic Compounds. Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology. Vol. 20B. 2000, Heidelberg: Springer. [ISBN 978-3-540-64968-7] (data for 3174 compounds) 374 pp, price EUR 4039, http://www.springer.com/laboe/book/978-3-540-64968-7
3Cc) Dykyj, J., J. Svoboda, R.C. Wilhoit, M. Frenkel, and Hall. K.R., Vapor Pressure and Antoine Constants for Nitrogen Containing Organic Compounds Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology. Vol. 20C. 2001, Heidelberg: Springer. [ISBN 978-3-540-41060-7] (data for 1575 compounds)197 pp, price EUR 2239, http://www.springer.com/laboe/book/978-3-540-41060-7

This vast compilation represents merge of TRC tables (see items 4x below) and Dykyj's two-volume book (3A and 3B) supplemented by selected literature data.

Data for over 9000 compounds are presented in form of parameters of Antoine eq or „extended“ Antoine eq, the approximate minimum and maximum temperatures covered by the data, the range of temperatures recommended for reliable use of the equation. The "rating" (consisting of letters A through D) indicates a rough order of reliability for the data used to develop the parameters: A - 0.1%; B -1%; C - 5%; D - 10%. The temperature of normal boiling point besides its own value serves as a check value.

To track the data used for generation of Antoine eq parameters is often impossible without access to TRC tables and/or Dykyj's books (items 3A and 3B)

4Aa) TRC Thermodynamic Tables – Hydrocarbons [ISBN: 1-883400-06-6]

4Ab) TRC Thermodynamic Tables Non-Hydrocarbons [ISBN: 1-883400-25-2] TRC-NH

Multiproperty tables containing evaluated data for 3700 compounds (TRC-H) and 3500 compounds (TRC-NH).

Paper form will be discontinued in 2009, for description of electronic version see 4B below.

4B) „Web Thermo Tables (WTT) - Professional Edition“ 7765 compounds
(http://www.nist.gov/srd/nistwebsub3.htm)

The Thermodynamics Research Center (formerly at Texas A&M University, now at NIST, Boulder, CO) has assembled, collected, evaluated and published tables of thermodynamic data from early forties. Among the properties covered by TRC Tables are vapor/sublimation pressures. . Tables contain constants derived from fitting experimental data with the Antoine and extended Antoine vapor pressure equations. The condensed phases can be either liquid or crystal. Thus, these constants provide evaluated vapor pressures which professional thermodynamicists believe represent the data within experimental error. Tables are regularly updated and can be purchased ~~in paper~~ or electronic form. Both accepted and rejected data sources are referenced for each datasheet covering usually several compounds; it is however not possible to see at glance which data sources were used for single compound. On the other hand the selection and datafitting is done very carefully and user can trust that selected data are best available. Only experimental data are used (no estimates). Data by GC technique are not covered.

Antoine eq is suitable to cover data for most of compounds in the pressure range from 1.5 kPa to 150 kPa. Extended Antoine eq can be used if higher pressures are available. When low-pressure data are available, To retain the Antoine equation for data below 1.5 kPa, a separate set of constants is fit to the low range data. The *TRC Thermodynamic Tables* use a least squares procedure that forces continuity in P and dP/dT for the same phase at the boundary.

Subscription for one year from USD 1200 (individual licence) to USD 2500 (organization with more than 2000 users) .

4C) TRC ThermoDataEngine (NIST Standard Reference Database 103)
(http://www.boulder.nist.gov/div838/trc/tde.html , USD 3790),

Multiproperty database including vapor pressures and sublimation pressures.

Either evaluated experimental data and/or estimated values supplied (in the case of vapor pressures, estimation method proposed by Ambrose and Walton is used (Ambrose, D. and J. Walton "Vapor pressures up to their critical temperature of normal alkanes and 1-alkanols." Pure and Applied Chemistry **61**(8) (1989): 1395-403).

4D) TRC Source database
600 000 numerical property values and their uncertainties on more than 17 200 pure compounds, 17 000 binary and ternary mixtures, and 4000 reaction systems.

4E) NIST WebBook Chemistry (NIST Standard Reference Database 69) (http://webbook.nist.gov/chemistry).
Multiproperty database, free of charge (as of spring 2008). Probably based on TRC Tables described above.

4D) Poling, B. E.; Prausnitz, J. M.; O'Connell, J. P. Properties of Gases and Liquids, 5th Ed., 768 pp., McGraw-Hill Professional Publishing: 2000. [ISBN:0-07-011682-2]

http://www.mcgraw-hill.co.uk/html/0071189718.html

Appendix A of this book contains parameters of Antoine and/or extended Antoine eq for selected compounds reproduced from TRC tables (items 4Aa and 4Ab above).

5A) DIPPR (Design Insitute for Physical Properties) Project 801 [Evaluated Process Design Data] (http://dippr.byu.edu)

Multiproperty tables cover evaluated data for almost 2000 compounds based on both experimental and estimated values. Vapour pressures and sublimation pressures are represented in the in the form of Riedel eqn parameters. Electronic version contains also original datapoints (including references) and accepted/rejected status for each datapoint. Data from TRC Tables, Boublik, and Dykyj (see items 2x, 3x, and 4x above) are frequently refitted to Riedel eqn. Acceptance of estimated values makes this source slightly less reliable than TRC. Price: from USD 750 to 2500 for local installation, USD 15000 to 26000 for network installation. Academic discounts available. Stand-alone or web access

6) Physical Property Data Service (PPDS3) (http://www.ppds.co.uk)

Simulation package containing multiproperty database covering data for approximately 1500 compounds. Price: on demand.

7Aa) Yaws C.L.: „Handbook of vapor pressure, Volume 1: C1 to C4compounds“

348 pp, Gulf, Houston 1994 [ISBN 0884151891]

7Ab) Yaws C.L.: „Handbook of vapor pressure,Volume 2: C5 to C7 Compounds“

367 compounds, 348 pp, Gulf, Houston 1994 [ISBN 0884151905]

7Ac) Yaws C.L.: „Handbook of vapor pressure,Volume 3: C8 to C28 Compounds“

363 compounds, 392 pp, Gulf, Houston 1994 [ISBN 0884151913] .

7Ad) Yaws C.L.: „Handbook of vapor pressure, Volume 4: Inorganic compounds and elements“
348 pp, Gulf, Houston 1995 [ISBN 0884151913]

Data presented graphically.

7B) Yaws C.L. „The Yaws handbook of vapor pressure : Antoine coefficients“
8200 compounds, 168 pp, USD 175. Gulf, Houston 2007 [ISBN 1-933762-10-1]
http://www.gulfpub.com/default.asp?Page=14&productid=8113&searchtype=2&ls=relatedproducts

8) **ESDU** ("Engineering Sciences Data Unit") http://en.wikipedia.org/wiki/ESDU ,
http://www.ihsesdu.com/cgi-bin/ps.pl?sess=unlicensed_1080506073328qrq&t=ser&p=pdce
2a Vapour pressure. General, aliphatic hydrocarbons
2b Vapour pressure. Aliphatic hydrocarbons (cont.).
2c Vapour pressure. Aromatic and cyclo compounds.
2d(i) Vapour pressure. Organic compounds containing oxygen.
2d(ii) Vapour pressure. Organic compounds containing oxygen (cont.).
2d(iii) Vapour pressure. Organic compounds containing oxygen (cont.).
2e Vapour pressure. Aliphatic compounds containing nitrogen.
2f(i) Vapour pressure. Halogenated aliphatic hydrocarbons.
2f(ii) Vapour pressure. Halogenated aromatic hydrocarbons.
2g Vapour pressure. Organic sulphur compounds.
2h Vapour pressure. Polycyclic compounds.
Price on demand. "3000+ compounds"

9a) Lide, D. R. *CRC handbook of chemistry and physics*. 88th Ed. CRC: Boca Raton, 2007. [ISBN 0849304881] $140. Multiproperty tables. Section 6 (Fluid properties) contains tables

- Sublimation Pressure of Solids (sublimation (vapor) pressure of 47 representative solids as a function of temperature)
- Vapor Pressure (vapor pressure data for about 1800 inorganic and organic substances. In order to accommodate elements and compounds ranging from refractory to highly volatile in a single table, the temperature at which the vapor pressure reaches specified pressure values is listed. The pressure values run in decade steps from 1 Pa (about 7.5 μm Hg) to 100 kPa (about 750 mm Hg).All temperatures are given in °C.)
- Vapor Pressure of Fluids at Temperatures below 300 K (vapor pressures of 67 important fluids in the temperature range 2 to 300 K).
- Vapor Pressure of Ice
- Vapor Pressure of Water from 0 to 370°C
- Boiling Point of Water at Various Pressures

- Vapor Pressure of Saturated Salt Solutions
- IUPAC Recommended Data for Vapor Pressure Calibration

http://www.crcpress.com/shopping_cart/products/product_detail.asp?sku=488&isbn=9780849304880&parent_id=&pc=

9b) http://www.hbcpnetbase.com
Internet version of 9a)

10) Lencka, M.; Szafranski, A.; Maczynski, A., *Verified vapor pressure data, Vol. 1: Organic Compounds Containing Nitrogen*. PWN-Polish Scientific Publishers: Warszawa, 1984. 403 pp[ISBN 83-01-05409-3] 386 datasets for 272 substances published over 1920-1981. Both original and SI values tabulated along with Antoine eq parameters.

11) Stephenson, R. M.; Malanowski, S.; Ambrose, D., *Handbook of the thermodynamics of organic compounds*. Elsevier: New York, 1987.

12) Dortmund Data Bank http://www.ddbst.de/new/DDB/frame_PCP.htm
This multiproperty database contains 29159 vapor pressure datasets for 7922 compounds (7733 references)

Besides the abovementioned sources related (mainly) with technological applications there are also resources linked with environmental chemistry. These works often covers vapour pressures along with other environmentally important properties as octanol-water patritiom coefficient, aqueous solubility, Henry's law constant etc. Unfortunately, values are frequently presented at 298.15 K only.

20Aa) Howard, P.H., W.F. Jarvis, G.W. Sage, D.K. Basu, A.D. Gray, W.M. Meylan, and E.K. Grosbie, Handbook of Environmental Fate and Exposure Data for Organic Chemicals. I. Large Production and Priority Pollutants. 1990, Chelsea, Michigan: Lewis Publishers 574 pp. [ISBN 0-87371-151-3]

20Ab) Howard, P.H., G.W. Sage, W.F. Jarvis, and D.A. Gray, Handbook of Environmental Fate and Exposure data for Organic Chemicals. II. Solvents. 1991, Chelsea, Michigan: Lewis Publishers, 546 pp. [ISBN 0-87371-204-8]

20Ac) Howard, P.H., E.M. Michalenko, W.F. Jarvis, D.K. Basu, G.W. Sage, J.A. Beauman, and D.A. Gray, Handbook of Environmental Fate and Exposure data for Organic Chemicals. III. Pesticides. 1991, Chelsea, Michigan: Lewis Publishers, 684 pp.

[ISBN 0-87371-328-1]

20Ad) Howard, P.H., E.M. Michalenko, D.K. Basu, G.W. Sage, W.M. Meylan, J.A. Beauman, W.F. Jarvis, and D.A. Gray, Handbook of Environmental Fate and Exposure data for Organic Chemicals. IV. Solvents 2. 1993, Chelsea, Michigan: Lewis Publishers, 578 pp. [ISBN 0-87371-413-X]

20Ae) Howard, P.H., G.W. Sage, E.M. Michalenko, D.K. Basu, A. Hill, and D. Aronson, Handbook of Environmental Fate and Exposure data for Organic Chemicals. V. Solvents 3. 1997, New York: CRC Lewis Publishers. 491 pp. [ISBN 0-87371-151-3]

Altogether this five-volume handbook covers data for nearly 400 compounds. Single (selected) value is given.

20B) Howard P.H. Handbook of Physical Properties of Organic Chemicals 1996, CRC Press,

$160, 2112 pp, [ISBN 1566702275] Multiproperty handbook. Single (selected) value of vapor pressure is given.
http://www.crcpress.com/shopping_cart/products/product_detail.asp?sku=L976

20C) Syracuse Research Corporation (SRC) is an independent, not-for-profit research and development organization http://www.syrres.com/esc/physdemo.htm

20D) http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm Free download. Module Mpbpwin calculates value of normal boiling point temperature and value of vapor pressure at 298.15 K (estimated and/or unreferenced experimental data are supplied)

21Aa) Mackay, D., W.Y. Shiu, and K.C. Ma, Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. I. Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. 1992, Lewis Publishers, Boca Raton 697 pp. [ISBN 0-87371-513-6]

21Ab) Mackay, D., W.Y. Shiu, and K.C. Ma, Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. II. Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins, and Dibenzofurans. 1992, Lewis Publishers, Boca Raton 597 pp. [ISBN 0-87371-583-7]

21Ac) Mackay, D., W.Y. Shiu, and K.C. Ma, Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. III. Volatile Organic Chemicals. 1993, Lewis Publishers, Boca Raton 916 pp. [ISBN 0-83731-973-5]

21Ad) Mackay, D., W.Y. Shiu, and K.C. Ma, Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. IV. Oxygen, Nitrogen, and Sulfur Containing Compounds. 1995, Lewis Publishers, Boca Raton 962 pp. [ISBN 1-56670-035-3]

21Ae) Mackay, D., W.Y. Shiu, and K.C. Ma, Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. V. Pesticide Chemicals. 1997, Lewis Publishers, Boca Raton 812 pp. [ISBN 1-56670-255-0]

Altogether this five-volume handbook covers data for over 700 compounds. All published values are presented (including „recommended“ values and estimations).

21Ba) Mackay D., Shiu W.Y., Ma K.-C., Lee, S.C. Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Taylor&Francis, Boca Raton, 2006 [ISBN 1-56670-687-4]

http://www.crcpress.com/shopping_cart/products/product_detail.asp?sku=L1687&isbn=9781566706872&parent_id=&pc=

Volume I. Introduction and Hydrocarbons;Volume II. Halogenated Hydrocarbons;Volume III. Oxygen Compounds; Volume IV. Nitrogen and Sulfur Compounds, Herbicides, Insekticides,Fungicides.
Four-volume enlarged reedition of 21A. Altogether 4216 pp and more than 1250 compounds, $1075,

21Bb) Mackay D., Shiu W.Y., Ma K.-C., Lee, S.C. Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Taylor&Francis, Boca Raton, 2006 [ISBN 0849388996]

http://www.crcpress.com/shopping_cart/products/product_detail.asp?sku=8899&isbn=9780849388996&parent_id=&pc=

Fully searchable CD version of 21Ba. $1075.

22) ACD Labs. http://www.acdlabs.com/products/phys_chem_lab/bp/capabilities.html

“To determine constants and relationships, our algorithm uses an **internal database** that contains boiling points for 10,000 compounds - 6,000 of which have boiling point values at 760 mmHg. The database values were also used to evaluate and fine-tune the specialized

algorithms for ACD/Boiling Point. **Your compound does not have to be in the database** in order to have its boiling point calculated. "

Values supplied by ACD Labs are available via electronic version of Chemical Abstracts (SciFinder)

Review papers in scientific journals.

50) Stull, D. R., Vapor pressure of pure substances. Organic compounds *Ind. Eng. Chem.* **1947,** 39, 517-40. Inorganic compounds *Ind. Eng. Chem.* **1947,** 39, 540-50. Correction. *Ind. Eng. Chem.* **1947,** 39, 1684.

Temperatures corresponding to selected vapor pressures in mm Hg (1, 5, 10, 20, 40, 60, 100, 200, 400, 760) tabulated. Extensive bibliography, data up to 1942 covered. Should not be used if newer data are available.

51) Jones, A. H., Sublimation-pressure data for organic compounds. *J. Chem. Eng. Data* **1960,** 5, (No. 2), 196-200.

Parameters of simples two-parameter eq for about 180 compounds are presented.

52) Ambrose, D. and J. Walton *"Vapor pressures up to their critical temperature of normal alkanes and 1-alkanols."* *Pure and Applied Chemistry* 61(8) (1989): 1395-403).

Critically evaluated vapor pressures presented in the form of Wagner eq parameters

53) Růžička, K. and Majer, V. Simultaneous Treatment of Vapor Pressures and Related Thermal Data Between the Triple and Normal Boiling Temperatures for *n*-Alkanes C_5-C_{20}. *J. Phys. Chem. Ref. Data* 1994, 23, 1-39.

Complement to Ambrose and Walton (item 52) with emphases to low-pressure region.

54) Lemmon, E. W. and A. R. H. Goodwin (2000). "Critical properties and vapor pressure equation for alkanes C_nH_{2n+2}: Normal alkanes with n <= 36 and isomers for n=4 through n=9." *J. Phys. Chem. Ref. Data* **29**(1): 1-39.

55) Delle Site, A. (1997). "The vapor pressure of environmentally significant organic chemicals: a review of methods and data at ambient temperature." *Journal of Physical and Chemical Reference Data* **26**(1): 157-193.

56A) Shiu, W.-Y. and K.-C. Ma (2000). "Temperature Dependence of Physical-Chemical Properties of Selected Chemicals of Environmental Interest. I. Mononuclear and Polynuclear Aromatic Hydrocarbons." *Journal of Physical and Chemical Reference Data* **29**(1): 41-130.

56B) Shiu, W.-Y. and K.-C. Ma (2000). "Temperature Dependence of Physical-Chemical Properties of Selected Chemicals of Environmental Interest. II. Chlorobenzenes, Polychlorinated Biphenyls, Polychlorinated Dibenzo-p-dioxins, and Dibenzofurans." *Journal of Physical and Chemical Reference Data* **29**(3): 387-462.

57A) Chickos, J. S. and W. E. Acree, Jr. (2002). "Enthalpies of sublimation of organic and organometallic compounds. 1910-2001." *Journal of Physical and Chemical Reference Data* **31**(2): 537-698.

57B) Chickos, J. S. and W. E. Acree, Jr. (2003). "Enthalpies of Vaporization of Organic and Organometallic Compounds, 1880-2002." *J.Phys.Chem.Ref.Data* **32**(2): 519-878.

Valuable source of bibliographic information for vapor pressures and sublimation pressures.

Appendix B: Reviews of experimental techniques for vapour pressure measurement

1) Ambrose, D., Vapor pressure. In *Experimental Thermodynamics of Non-reacting Systems*, Le Neindre, B.; Vodar, B., Eds. Butterworths: London, 1975; pp 607-656. [ISBN 0408705663].

2) Carson, A. S., The measurement of vapor pressure. In *Thermochemistry and Its Applications to Chemical and Biochemical Systems*, Ribeiro da Silva, M. A. V., Ed., D.Riedel Publishing Company: 1984; pp 127-41. [ISBN 978-9027716989]

3) Verevkin, S. P., Phase Changes in Pure Component Systems: Liquids and Gases. In *Measurement of the Thermodynamic Properties of Multiple Phases,* Weir, R. D.; de Loos, T. W., Eds. Elsevier: Amsterdam, 2005; pp 5-30. [ISBN 0444519777].

4) Delle Site, A., The vapor pressure of environmentally significant organic chemicals: a review of methods and data at ambient temperature. Journal of Physical and Chemical Reference Data 1997, 26, (1), 157-193.