Supplementary Material to "The critical assessment of vapour pressure estimation methods for use in modelling the formation of atmospheric organic aerosol" by Mark H Barley and Gordon McFiggans.

In the first part of this Supplementary material the data sources for Test Set 1 and Test Set 2 are listed (see Table 1 and Table 2). The second part describes the calculation of subcooled liquid vapour pressures for those compounds in Test Set 2 for which solid (sublimation) vapour pressures were measured.

PART 1

Table 1:- Data sources for the compounds of Test Set 1

	T_m[a]	T_b[a]	Vapour Pressure data
2-Octanone	[1]	[2][b]	[1]
Limonene		[3][b]	[3]
Linalool	???[c]	[4, 5][d]	[3]
n-Decanal		[6]	[7]
Cyclohexyl Formate	[8]	[9][e]	[10]
1-Methyl-2-nitrobenzene		[11]	[12]
2-Butanone		[13]	[2]
Propylbenzene		[13]	[14]
Hexanoic acid	[15]	[16]	[17, 18]
Heptanoic acid	[19]	[16]	[17, 18]
Benzyl alcohol	[20]	[21]	[22, 23]
Phenethyl alcohol		[11]	[24]
3-Methyl phenol	[25]	[13]	[26]
2-Ethyl phenol		[13]	[27]
1,2 Ethanediol		[13]	[28, 29]
1,6 Hexanediol	[30]	[31]	[31, 32]
1,2,3-Propanetriol (Glycerol)	[15]	[33]	[34]
1,1'-oxobisethane (Diethylether)		[13]	[35]
1,1'-oxobisbenzene (Diphenylether)	[20]	[13]	[36]
Octanenitrile		[37][b]	[38]
Anisaldehyde	[39]	[40][f]	[41]
1,2-Dichlorobenzene		[13]	[42]

Notes:-a) Melting point (T_m) from Detherm/DDB unless otherwise indicated; normal boiling point (T_b) from primary literature. b) T_b obtained by interpolation of vapour pressure data. c) T_m unknown but low (below 273K). d) T_b quoted by ref. 4 supported by extrapolating vapour pressure data in ref. 5 (T_b agree within 1K). e) T_b obtained by extrapolating vapour pressure data-(from P = 99800Pa). f) T_b obtained by extrapolating vapour pressure data- (from 100000Pa).

Table 2:- Data sources for the compounds of Test Set 2

	Vapour pressure data	Melting point (T_m)
1,2,3-Trihydroxypropane (Glycerol)	[34]	[20]
1,2-Pentanediol	[43]	??[a]
1,4-Butanediol	[44]	[45]
2-Aminoethanol	[46]	[46]
2-Aminonitrobenzene	[47]	[48]
2-Chloropropionic acid	[49]	[49]
2-(Methylamino)ethanol	[46]	??[a,b]
2-Phenylbromide-TEGMME[c]	[50]	??[a]
2,4-Pentanediol	[51]	??[a]
2,6-Dinitrotoluene	[52]	[53]
2-Chloro-3,5 Dimethoxy,4-hydroxybenzaldehyde[d]	[54]	[55]
2-Hydroxybenzoic acid	[56]	[48]
3-(2-Methoxyphenyl)propionic acid	[57]	[57]
3-(3,4-Dimethoxyphenyl)propionic acid	[57]	[57]
3,4-Dichloronitrobenzene	[58]	[58]
3,4-dihydroxychlorobenzene[d]	[54]	[59]
3,5-di-t-Butylcatechol	[60]	[60]
3,7-Dimethyl-7-hydroxyoctanal	[41, 61]	??[e]
3-Chloro-2,6 Dimethoxyphenol[d]	[54]	[55]
3-Chloroaminobenzene	[58]	[58]
3-Hydroxypropanenitrile	[62]	[63]
3-Nitro-3-(4-nitrophenyl)-pentane	[47]	??[a]
3-Nitrobenzoic acid	[64]	[48]
4-Aminobenzoic acid	[65]	[48, 66]
3-Nitrophenol	[67]	[67]
Anisaldehyde	[41, 61]	[39]
Benzyl Salicylate	[41, 61]	[41]
Dibutylphthalate	[68]	[69]
Ethyl vanillin	[61, 70]	[71]
Eugenol	[61, 72]	[63]
Glutaric Acid	[73]	[74]
Glycerine carbonate	[75]	??[a]
Heliotropin	[61, 70]	[61]
iso-Amyl Salicylate	[41, 61]	??[f]
Ketol	[76]	[76]
Methyl Anthranilate	[61, 77]	[61, 77]
Musk Ambrette	[61, 70]	[61, 70]
N-methyldiethanolamine	[78]	??[a, g]
p-Acetylanisole	[77]	[77]
Phloroglucinol	[79]	[80]
Pimelic Acid	[73]	[74]
Tetraethylene glycol	[29]	[63]
Triacetin	[81]	[63]
Triethylene glycol dinitrate	[81]	??[a,h]

Notes:- a) T_m unknown but from the vapour pressure source it is clear that the measurements were made on a liquid. b) Primary source for T_m not found but probably 269K. c) Full name (2-Phenylbromide) triethylene glycol monomethyl ether. d) Vapour pressure measurements by GC method- values obtained are sub-cooled liquid values so no correction required. e) T_m unknown but there is no inflection in the vapour pressure curve (283-333K) and a refractive index at 293.15K is quoted. f) T_m unknown but there is no inflection in the vapour pressure curve (288-328 K) and n-alkane salicylates (up to C6) all have T_m < 280K. g) Primary source for T_m not found but probably 252K. h) Primary source for T_m not found but probably 254K.

PART 2:- The Correction of Solid Vapour Pressures to Subcooled Liquid Vapour Pressures.

For those compounds where the measured vapour pressures are that of the solid (see Table 3 in the paper) the corresponding sub-cooled liquid vapour pressures (SCL-VP) were obtained by applying the correction of Prausnitz[82]

$$Ln(P_i^o) = Ln(P_{SCL}) = Ln(P_S) - \frac{\Delta S_{fus}}{R}\left(1 - \frac{T_m}{T}\right) - \frac{\Delta C_p}{RT}\left(T_m - T\right) + \frac{\Delta C_p}{R} Ln\left(\frac{T_m}{T}\right) \quad \text{Eq. 1}$$

Where P_{SCL} and P_S are the SCL-VP and experimental solid (sublimation) vapour pressure (in atmospheres) respectively; ΔS_{fus} is the entropy of fusion; ΔC_p is the best estimate of the underlying change in heat capacity between the liquid and solid state at the melting point; and T_m is the melting point temperature (used instead of the triple point temperature).

If T_m-T was less than 30K then the last two terms were ignored and an estimated ΔS_{fus} (using the method of Myrdal and Yalkowski [83]) could be used. If T_m-T was greater than 30K then an experimentally derived ΔS_{fus} had to be used and the heat capacity terms were included with heat capacity data for the liquid and vapour phases obtained from experimental data (if available) or estimated[84, 85]. Table 3 (below) shows the effect of the first term in the above equation on the correction of measured solid vapour pressures. The references provided with the ΔS_{fus} values refer to experimental determinations of the enthalpy of fusion (ΔH_{fus}) with ΔS_{fus} calculated by:-

$$\Delta S_{fus} = \Delta H_{fus} / T_m$$

Table 3:- The correction of solid vapour pressures using the first term of the Prausnitz equation (Eq. 1 above)

Compound (Solid)	T_m(K)	T-range (K)	P-range (Pa)	ΔS_{fus} [a]	Corrected P-range(Pa)
2-Aminonitrobenzene	342.5	313.5-342.3	0.71-12.33	47.04[48]	1.20-12.37
2,6-Dinitrotoluene	329.6	277.15-323.15	0.00342-1.718	58.50[53]	0.0129-1.974
2-Hydroxybenzoic acid	431.8	307.05-323.71	0.0682-0.468	56.97[48]	1.103-4.611
3-(2-MP)PA[b]	360.5	331.56-347.165	0.1556-1.0957	70.27[57]	0.329-1.514
3-(3,4-DMP)PA[b]	370.9	352.18-366.16	0.0664-0.4115	87.31[57]	0.116-0.471
3,5-di-t-Butylcatechol	372.8	313.2-346.2	0.0732-3.17	64.65[60]	0.321-5.761
3-Nitrobenzoic acid	413	347.16-361.16	0.215-0.905	51.82[48, 86]	0.700-2.21
3-Nitrophenol	370.0	357.2-369.3	12.05-35.13	46.76[67]	14.74-35.51
4-Aminobenzoic acid	461.4	359.14-382.56	0.1-1.0	45.3[48]	0.47-3.07
Ethyl vanillin	351.2	323.35-337.45	0.47-2.75	72.45[71]	0.96-3.78
Glutaric Acid	371	348.15-363.15	0.22-1.2	62.0[74]	0.359-1.410
Heliotropin[c]	310.2	293.45-308.45	0.39-2.20	56.5 (est)	0.579-2.28
Musk Ambrette	358.2	328.55-345.45	0.141-0.973	70.3 (est)	0.303-1.33
Phloroglucinol	491.8	381.31-404.58	0.1-1.0	70.15[80]	1.152-6.164
Pimelic Acid	377.5	358.15-371.66	0.126-0.67	80.26[74]	0.212-0.786

Notes:- a) DelS(fus) in J/mole.K. b) 3-(2-MP)PA = 3-(2-Methoxyphenyl)propionic acid; 3-(3,4-DMP)PA = 3-(3,4-Dimethoxyphenyl)propionic acid. c) For Heliotropin correction applied to 7 points below melting point.

For those compounds with experimental data at temperatures more than 30K below the melting point all three terms of Eq. 1 were used. Table 4 summarises the details of the derivation of liquid and solid heat capacity for each of the compounds and the corresponding correction to the vapour pressure. This additional correction was usually very small compared to that shown in Table 3 but for two compounds (phloroglucinol and 2-hydroxybenzoic acid) it was quite significant.

Table 4 The effect of heat capacities on the calculation of SCL-VP data.

			<======J/mole.K======>			
Compound	**T-Range (K)**	**P-Range (Pa) (From Table 3)**	**C_p(s)**	**C_p(l)**	**ΔC_p**	**P-Range (Pa) (SCL-VP)**
2,6-Dinitrotoluene[b]	277.15-323.15	0.0129-1.974	246[53][a]	253.7[53][a]	7.7	0.0127-1.974
2-Hydroxybenzoic acid	307.05-323.71	1.103-4.611	214.7[87][d,e]	330.7[c]	116.1	0.443-2.434
3,5-di-t-Butylcatechol	313.2-346.2	0.321-5.761	455.0[d]	549.3[c]	94.3	0.270-5.58
3-Nitrobenzoic acid	347.16-361.16	0.700-2.21	236.9[88][d,e]	313.5[c]	76.6	0.604-2.03
4-Aminobenzoic acid	359.14-382.56	0.47-3.07	211.3[d]	337.3[c]	126	0.28-2.31
Phloroglucinol	381.31-404.58	1.152-6.164	217.1[d]	297.7[c]	80.6	0.8185-5.060
Pimelic Acid	358.15-371.66	0.212-0.786	364.9[74]	376.8[74]	11.9	0.212-0.786

Notes:- a) Short (<10K) extrapolation of experimental data; b) Form A- see Finch and Payne[53]; c) Cp(l) estimated by the method of Ruzicka and Domalski[84, 85]; d) Cp(s) estimated by the power law of Goodman[85]; e) A- parameter in Goodman power law fitted to experimental heat capacity data.

References

1. Covarrubias-Cervantes, M., et al., *Saturated vapour pressure of aroma compounds at various temperatures.* Food Chemistry, 2004. **85**(2): p. 221-229.
2. Guetachew, T., et al., *Vapor pressures and sublimation pressures of naphthalene and of five alkan-2-ones (C4, C5, C7, C8, C9) at pressures in the range from 0.3 Pa to 160 kPa.* . ELDATA International Electronic Journal of Physical Chemistry Reference Data, 1995. **1**: p. 249-254.
3. Espinosa Diaz, M.A., et al., *Experimental and estimated saturated vapour pressures of aroma compounds.* Fluid Phase Equilibria, 1999. **157**: p. 257-270.
4. Zaretskii, M.I., et al., Z Prikl. Khim., 1999. **72**: p. 1433-1436.
5. Deng, D.S., H.R. Li, and S.J. Han, *Isobaric (vapour plus liquid) equilibria of (linalool+1propanol) and (linalool+1butanol).* Journal of Chemical Thermodynamics, 2002. **34**(9): p. 1431-1437.
6. Dyakova, G.N., et al., *Investigation of the Vapor-Pressures of Aliphatic-Aldehydes.* Journal of Applied Chemistry of the Ussr, 1981. **54**(7): p. 1413-1415.
7. Verevkin, S.P., et al., *Vapor pressures and enthalpies of vaporization of a series of the linear aliphatic aldehydes.* Fluid Phase Equilibria, 2003. **206**(1-2): p. 331-339.
8. Kozyro, A.A., et al., *Thermodynamic properties of some cyclohexyl esters in the condensed state.* Journal of Chemical Thermodynamics, 2001. **33**(3): p. 305-331.
9. Steyer, F. and K. Sundmacher, *VLE and LLE data set for the system cyclohexane plus cyclohexene plus water plus cyclohexanol plus formic acid*

plus formic acid cyclohexyl ester. Journal of Chemical and Engineering Data, 2005. **50**(4): p. 1277-1282.
10. Zaitsau, D.H., et al., *Comprehensive study of vapor pressures and enthalpies of vaporization of cyclohexyl esters.* Journal of Chemical and Engineering Data, 2003. **48**(6): p. 1393-1400.
11. Dreisbach, R.R. and S.A. Shrader, *Vapor Pressure Temperature Data on Some Organic Compounds.* Industrial and Engineering Chemistry, 1949. **41**(12): p. 2879-2880.
12. Verevkin, S.P. and A. Heintz, *Thermochemistry of substituted benzenes: quantification of ortho-, para-, meta-, and buttress interactions in alkyl-substituted nitrobenzenes.* Journal of Chemical Thermodynamics, 2000. **32**(9): p. 1169-1182.
13. Ambrose, D. and R. Townsend, *Vapour-Liquid Critical Properties*, in *NPL Report*. 1977.
14. Ruzicka, V., et al., *Vapor-Pressures for a Group of High-Boiling Alkylbenzenes under Environmental-Conditions.* Thermochimica Acta, 1994. **245**: p. 121-144.
15. Costello, J.M. and S.T. Bowden, *The Temperature Variation of Orthobaric Density Difference in Liquid-Vapour Systems .4. Fatty Acids.* Recueil Des Travaux Chimiques Des Pays-Bas-Journal of the Royal Netherlands Chemical Society, 1958. **77**(8): p. 803-810.
16. Pool, W.O. and A.W. Ralston, *Boiling points of N-alkyl acids.* Ind. Eng. Chem., 1942. **34**: p. 1104-5.
17. Dekruif, C.G. and H.A.J. Oonk, *Enthalpies of Vaporization and Vapor-Pressures of 7 Aliphatic Carboxylic-Acids.* Journal of Chemical Thermodynamics, 1979. **11**(3): p. 287-290.
18. Verevkin, S.P., *Measurement and prediction of the monocarboxylic acids thermochemical properties.* Journal of Chemical and Engineering Data, 2000. **45**(5): p. 953-960.
19. Adriaanse, N., H. Dekker, and J. Coops, *Some Physical Constants of Normal Saturated Fatty Acids + Their Methyl Esters.* Recueil Des Travaux Chimiques Des Pays-Bas-Journal of the Royal Netherlands Chemical Society, 1964. **83**(6): p. 557-572.
20. Domalski, E.S., W.H. Evans, and E.D. Hearing, *Heat capacities and entropies of organic compounds in the condensed phase.* . Journal of Physical Chemistry Reference data (supplement 1), 1984. **13**(1): p. 1-286.
21. Ambrose, D. and N.B. Ghiassee, *Vapor-Pressures, Critical-Temperatures, and Critical Pressures of Benzyl Alcohol, Octan-2-Ol, and 2-Ethylhexan-1-Ol.* Journal of Chemical Thermodynamics, 1990. **22**(3): p. 307-311.
22. Verevkin, S.P., *Strain effects in phenyl-substituted methanes. Geminal interaction between phenyl and the electron-releasing substituent in benzylamines and benzyl alcohols.* Journal of Chemical and Engineering Data, 1999. **44**(6): p. 1245-1251.
23. Apelblat, A., A. Tamir, and M. Wagner, *Excess Gibbs Energy of (Formic-Acid + Benzyl Alcohol) and (Acetic-Acid + Benzyl Alcohol).* Journal of Chemical Thermodynamics, 1984. **16**(9): p. 891-895.
24. Serpinskii, V.V., S.A. Voitkevich, and N.Y. Lyuboshits, *Opredelenie Davleniya Nasyshchennogo Para Nekotorykh Dushistykh Veshchestv .2.* Zhurnal Fizicheskoi Khimii, 1954. **28**(5): p. 810-813.

25. Lee, L.S., C.W. Lin, and C.H. Kao, *Using tert-butyl alcohol as an adductive agent for separation of an m-cresol and 2,6-xylenol mixture.* Industrial & Engineering Chemistry Research, 2000. **39**(6): p. 2068-2075.
26. Biddiscombe, D.P. and J.F. Martin, *Vapour Pressures of Phenol and the Cresols.* Transactions of the Faraday Society, 1958. **54**(9): p. 1316-1322.
27. Biddiscombe, D.P., et al., *Thermodynamic Properties of Organic Oxygen Compounds .13. Preparation and Physical Properties of Pure Ethylphenols.* Journal of the Chemical Society, 1963(Dec): p. 5764-5768.
28. Mokbel, I., et al., *Static measurements of the total vapor pressure of ethane-1,2-diol + water mixtures at temperatures from 258 K to 363 K.* ELDATA International Electronic Journal of Physico-Chemical Reference Data, 1999. **5**: p. 79-84.
29. Hales, J.L., R.C. Cogman, and W.J. Frith, *A Transpiration-Glc Apparatus for Measurement of Low Vapor Concentration.* Journal of Chemical Thermodynamics, 1981. **13**(6): p. 591-601.
30. Knauth, P. and R. Sabbah, *Energetics of Intramolecular and Intermolecular Bonds in Omega-Alkanediols .3. Thermochemical Study of 1,6-Hexanediol, 1,7-Heptanediol, 1,8-Octanediol, 1,9-Nonanediol, and 1,10-Decanediol at 298.15K.* Canadian Journal of Chemistry-Revue Canadienne De Chimie, 1990. **68**(5): p. 731-734.
31. Steele, W.V., et al., *Thermodynamic properties and ideal-gas enthalpies of formation for butyl vinyl ether, 1,2-dimethoxyethane, methyl glycolate, bicyclo[2.2.1]hept-2-ene, 5-vinylbicyclo[2,2.1]hept-2-ene, trans-azobenzene, butyl acrylate, di-tert-butyl ether, and hexane-1,6-diol.* Journal of Chemical and Engineering Data, 1996. **41**(6): p. 1285-1302.
32. Piacente, V., D. Ferro, and G. Dellagatta, *Vaporization Enthalpies of a Series of Alpha,Omega-Alkanediols from Vapor-Pressure Measurements.* Thermochimica Acta, 1993. **223**: p. 65-73.
33. Sokolov, N.M., et al., *Separation of a 1,2-propylene glycol-ethylene glycol mixture at different pressures.* Khimicheskaya Promyshlennost (Moscow, Russian Federation) 1972. **48**(7): p. 499-501.
34. Cammenga, H.K., F.W. Schulze, and W. Theuerl, *Vapor-Pressure and Evaporation Coefficient of Glycerol.* Journal of Chemical and Engineering Data, 1977. **22**(2): p. 131-134.
35. Drucker, C., E. Jimeno, and W. Kangro, *Vapor pressure of liquids at low temperatures.* . Z physik. Chem. (Leipzig), 1915. **90**: p. 513-552.
36. Bent, H.E. and R.J. Francel, *The Vapor Pressure of Mustard Gas (Beta,Beta+-Dichloroethylsulfide), Diphenyl Ether and Their Mixtures.* Journal of the American Chemical Society, 1948. **70**(2): p. 634-637.
37. Meyer, E.F., T.A. Renner, and K.S. Stec, *Cohesive Energies in Polar Organic Liquids .2. Alkyl Nitriles and 1-Chloroalkanes.* Journal of Physical Chemistry, 1971. **75**(5): p. 642-8.
38. Emel'yanenko, V.N., et al., *Vapour pressures and enthalpies of vapourization of a series of the linear aliphatic nitriles.* Journal of Chemical Thermodynamics, 2005. **37**(1): p. 73-81.
39. Kendall, J., W.A. Gibbons, and *The addition compounds of aldehydes and ketones with organic acids.* Journal of the American Chemical Society, 1915. **37**: p. 149-162.
40. Scholz, A.G.R. and E. Brunner, *Isobaric Vapor-Liquid-Equilibria of the Binary-Systems Consisting of Anisaldehyde, Methyl Anisate, and Anisyl*

Alcohol at 2-Kpa. Journal of Chemical and Engineering Data, 1985. **30**(1): p. 72-74.
41. Serpinskii, V.V., S.A. Voitkevich, and N.Y. Lyuboshits, *Determination of Saturated Vapour Pressure of Some Anomatic Principles.* Zhurnal Fizicheskoi Khimii, 1955. **29**(4): p. 653-657.
42. Polednicek, M., et al., *Vapor pressures and sublimation pressures of dichlorobenzenes (1,2-, 1, 3-, 1,4-), trichlorobenzenes (1,2,3- and 1,3,5-), and pentachlorobenzene.* ELDATA International Electronic Journal of Physico-Chemical Data, 1996. **2**: p. 41-50.
43. Verevkin, S.P., *Determination of vapor pressures and enthalpies of vaporization of 1,2-alkanediols.* Fluid Phase Equilibria, 2004. **224**(1): p. 23-29.
44. Vasiltsova, T.V., et al., *Thermodynamic properties of mixtures containing ionic liquids. Activity coefficients of ethers and alcohols in 1-methyl-3-ethyl-imidazolium bis(trifluoromethyl-sulfonyl) imide using the transpiration method.* Journal of Chemical and Engineering Data, 2005. **50**(1): p. 142-148.
45. Lee, M.J., F.L. Wu, and H.M. Lin, *Separation of closely boiling compounds of catechol and 4-methoxyphenol with the aid of 1,4-butanediol.* Industrial & Engineering Chemistry Research, 2001. **40**(21): p. 4596-4602.
46. Kapteina, S., et al., *Vapor pressures and vaporization enthalpies of a series of ethanolamines.* Journal of Chemical and Engineering Data, 2005. **50**(2): p. 398-402.
47. Verevkin, S.P., *Thermochemistry of nitro compounds. Experimental standard enthalpies of formation and improved group-additivity values.* Thermochimica Acta, 1997. **307**(1): p. 17-25.
48. Domalski, E.S. and E.D. Hearing, *Heat Capacities and Entropies of Organic Compounds in the Condensed Phase. Volume III.* J Physical and Chemical Reference Data, 2006. **25**: p. 1-525.
49. Lagoa, A.L.C., et al., *Energetics of the C-Cl bond in CH3CH(Cl)COOH. Enthalpy of formation of (S)-(-)-2-chloropropionic acid and of the 1-carboxyethyl radical.* Journal of Physical Chemistry A, 2002. **106**(42): p. 9855-9861.
50. Dabrowska, A., A. Sporzynski, and S.P. Verevkin, *Vapour pressures and enthalpies of vaporization of a series of aromatic ethers of mono-, di- and triethylene glycol.* Fluid Phase Equilibria, 2006. **249**(1-2): p. 115-119.
51. Verevkin, S.P., *Vapor pressures and enthalpies of vaporization of a series of the 1,3-alkanediols.* Journal of Chemical and Engineering Data, 2007. **52**(1): p. 301-308.
52. Pella, P.A., *Measurement of Vapor-Pressures of Tnt, 2,4-Dnt, 2,6-Dnt, and Egdn.* Journal of Chemical Thermodynamics, 1977. **9**(4): p. 301-305.
53. Finch, A. and J. Payne, *Thermochemical Study of 2,6-Dinitrotoluene.* Thermochimica Acta, 1990. **164**: p. 55-63.
54. Lei, Y.D., et al., *Temperature dependent vapor pressures of chlorinated catechols, syringols, and syringaldehydes.* Journal of Chemical and Engineering Data, 1999. **44**(2): p. 200-202.
55. Varhanickova, D., et al., *Aqueous Solubilities of Chlorocatechols, Chlorovanillins, Chlorosyringols, and Chlorosyringaldeydes at 25-Degrees-C.* Journal of Chemical and Engineering Data, 1995. **40**(3): p. 620-622.
56. Colomina, M., et al., *Propiedades termoquimicas de derivados del acido benzoico.* Anales de Quimica, 1981. **77**: p. 114-117.

57. Monte, M.J.S. and D.M. Hillesheim, *Thermodynamic study on the sublimation of 3-phenylpropionic acid and of three methoxy-substituted 3-phenylpropionic acids.* Journal of Chemical Thermodynamics, 2001. **33**(8): p. 837-847.
58. Verevkin, S.P. and C. Schick, *Determination of vapor pressures, enthalpies of sublimation, enthalpies of vaporization, and enthalpies of fusion of a series of chloro-aminobenzenes and chloro-nitrobenzenes.* Fluid Phase Equilibria, 2003. **211**(2): p. 161-177.
59. Parke, D.V. and R.T. Williams, *Studies in Detoxication .63. Metabolism of Halogenobenzenes .A. Meta-Dichlorobenzene .B. Further Observations on the Metabolism of Chlorobenzene.* Biochemical Journal, 1955. **59**(3): p. 415-422.
60. Verevkin, S.P. and C. Schick, *Substituent effects on the benzene ring. Determination of the intramolecular interactions of substituents in tert-alkyl-substituted catechols from thermochemical measurements.* Journal of Chemical and Engineering Data, 2000. **45**(5): p. 946-952.
61. Serpinskii, V.V., S.A. Voitkevich, and N.Y. Lyuboshits, *Results of determination of pressures of saturated vapor of 36 Aromatic substances.* Trudy Vsesoyuz. Nauch.-Issledovatel. Inst. Sintet.i Natural. Dushishtykh Veshchestv., 1958. **4**: p. 125-130.
62. Roux, M., et al., *Experimental and computational thermochemical study of 3-hydroxypropanenitrile.* Journal of Chemical Thermodynamics, 2007. **39**(10): p. 1377-1383.
63. Dykyi, J., M. Repas, and *Saturation Vapor Pressure of Organic Compounds*. 1979: Veda Vydavatelstvo Slovenskej Akademie Vied, Bratislava
64. Ribeiro da Silva, M.A.V.R., et al., *Enthalpies of combustion, vapour pressures, and enthalpies of sublimation of three methoxy-nitrobenzoic acids. Vapour pressures and enthalpies of sublimation of the three nitrobenzoic acids.* Journal of Chemical Thermodynamics, 1999. **31**(11): p. 1429-1441.
65. Dekruif, C.G., J. Voogd, and J.C.A. Offringa, *Enthalpies of Sublimation and Vapor-Pressures of 14 Amino-Acids and Peptides.* Journal of Chemical Thermodynamics, 1979. **11**(7): p. 651-656.
66. Andrews, D.H., G. Lynn, and J. Johnson, *The heat capacities and heat of crystallization of some isomeric aromatic compounds.* J Am Chem Soc, 1926. **48**(5): p. 1274-1287.
67. Heintz, A., S. Kapteina, and S.P. Verevkin, *Pairwise-substitution effects and intramolecular hydrogen bonds in nitrophenols and methylnitrophenols. Thermochemical measurements and ab initio calculations.* Journal of Physical Chemistry A, 2007. **111**(28): p. 6552-6562.
68. Birks, J. and R.S. Bradley, *The Rate of Evaporation of Droplets .2. The Influence of Changes of Temperature and of the Surrounding Gas on the Rate of Evaporation of Drops of Di-Normal-Butyl Phthalate.* Proceedings of the Royal Society of London Series a-Mathematical and Physical Sciences, 1949. **198**(1053): p. 226-239.
69. Song, W.L., A. Li, and X.Q. Xu, *Water solubility enhancement of phthalates by cetyltrimethylammonium bromide and beta-cyclodextrin.* Industrial & Engineering Chemistry Research, 2003. **42**(5): p. 949-955.
70. Serpinskii, V.V., S.A. Voitkevich, and N.Y. Lyuboshits, *Determination of Saturated vapour pressures of Fragrances.* Zhurnal Fizicheskoi Khimii, 1953. **27**: p. 1032-38.

71. Skerget, M., et al., *Influence of the aromatic ring substituents on phase equilibria of vanillins in binary systems with CO2.* Fluid Phase Equilibria, 2005. **231**(1): p. 11-19.
72. Serpinskii, V.V., S.A. Voitkevich, and N.Y. Lyuboshitz, *Determination of the Saturated Vapor Pressures of Some Odorous Substances .6.* Zhurnal Fizicheskoi Khimii, 1957. **31**(6): p. 1278-1284.
73. Ribeiro da Silva, M.A.V., M.J.S. Monte, and J.R. Ribeiro, *Vapour pressures and the enthalpies and entropies of sublimation of five dicarboxylic acids.* Journal of Chemical Thermodynamics, 1999. **31**(8): p. 1093-1107.
74. Steele, W.V., et al., *Thermodynamic properties and ideal-gas enthalpies of formation for 1,4 diisopropylbenzene,1,2,4,5-tetraisoprophylbenzene, cyclohexanone oxime, dimethyl malonate, glutaric acid and pimelic acid.* Journal of Chemical and Engineering Data, 2002. **47**(4): p. 725-739.
75. Verevkin, S.P., et al., *Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates.* Fluid Phase Equilibria, 2008. **268**(1-2): p. 1-6.
76. Shevelyova, M.P., et al., *Thermodynamics of 2-(1 '-hydroxycyclohexyl)cyclohexanone: Vaporization, sublimation, and the ideal gas state thermodynamic properties.* Journal of Chemical and Engineering Data, 2006. **51**(5): p. 1946-1952.
77. Serpinskii, V.V., S.A. Voitkevich, and N.Y. Lyuboshits, *Opredelenie Davleniya Nasyshchennogo Para Nekotorykh Dushistykh Veshchestv .3.* Zhurnal Fizicheskoi Khimii, 1954. **28**(11): p. 1969-1974.
78. Noll, O., et al., *Vapor pressures and liquid densities of N-methylethanolamine, diethanolamine, and N-methyldiethanolamine.* . ELDATA: The International Electronic Journal of Physico-Chemical Data, 1998. **4**(3): p. 105-120.
79. Dewit, H.G.M., et al., *Vapor-Pressures and Lattice Energies of Oxalic-Acid, Mesotartaric Acid, Phloroglucinol, Myoinositol, and Their Hydrates.* Journal of Chemical Physics, 1983. **78**(3): p. 1470-1475.
80. Verevkin, S.P. and C. Schick, *Determination of vapor pressures, enthalpies of sublimation, and enthalpies of fusion of benzenetriols.* Thermochimica Acta, 2004. **415**(1-2): p. 35-42.
81. Woodman, A.L. and A. Adicoff, *Vapor Pressure of Triacetin, Triethylene glycol dinitrate and Metriol trinitrate.* J Chem Eng Data, 1963. **8**: p. 241-242.
82. Prausnitz, J.M., R.N. Lichtenhaler, and E.G. de Azevedo, *Molecular Thermodynamics of Fluid-Phase Equilibria*. 2nd ed. 1986, Englewood Cliffs, N J, USA: Prentice-Hall.
83. Myrdal, P.B. and S.H. Yalkowsky, *Estimating pure component vapor pressures of complex organic molecules.* Industrial & Engineering Chemistry Research, 1997. **36**(6): p. 2494-2499.
84. Ruzicka, V. and E.S. Domalski, *Estimation of the Heat-Capacities of Organic Liquids as a Function of Temperature Using Group Additivity .2. Compounds of Carbon, Hydrogen, Halogens, Nitrogen, Oxygen, and Sulfur.* Journal of Physical and Chemical Reference Data, 1993. **22**(3): p. 619-657.
85. Goodman, B.T., et al., *Use of the DIPPR database for development of quantitative structure-property relationship correlations: Heat capacity of solid organic compounds.* Journal of Chemical and Engineering Data, 2004. **49**(1): p. 24-31.
86. Rai, U.S. and K.D. Mandal, *Chemistry of Organic Eutectics - Para-Phenylenediamine-M-Nitrobenzoic Acid System Involving the 1-2 Addition*

Compound. Bulletin of the Chemical Society of Japan, 1990. **63**(5): p. 1496-1502.
87. Parks, G.S. and D.W. Light, *Thermal data on organic compounds. XIII. The heat capacities and entropies of n-tetradecane and the hydroxybenzoic acids. The relative free energies of some benzenoid position isomers.* Journal of the American Chemical Society, 1934. **56**: p. 1511-1513.
88. Andrews, D.H., *The specific heats of some isomers of the type ortho, meta and para C6H4XY from 110 to 340 K*
Journal of the American Chemical Society, 1926. **48**: p. 1287-1299.