Supplementary Material. Pankow and Asher (2007) "SIMPOL.1: A Simple Group Contribution Method for Predicting Vapor Pressures and Enthalpies of Vaporization of Multifunctional Organic Compounds", *Atmospheric Chemistry and Physics Discussions*.

Functional Form of Vapor Pressure Parameterizations and Data Sources

1. When utilized in this work, the form of the Antoine parameterization is that described by Reid *et al*. (1987):

$$p_{\mathrm{L}}^{\mathrm{o}}(\mathrm{atm}) = 0.9869 \times 10^{\beta} \qquad (1.1)$$

$$\beta = A - B(T + C)^{-1} \qquad (1.2)$$

The values of the coefficients *A*, *B*, and *C* utilized were found, or derived in this work, using the sources given in Sections 1.1–1.22. In the case of coefficients derived in this work, these were determined from experimental vapor pressures by minimizing the goodness-of-fit function

$$\chi^2 = \sum_{n=1}^{N_{\mathrm{T}}} \left[\beta(T_n) - \log\left(p_{\exp}(T_n) \right) \right]^2 \qquad (1.3)$$

where $p_{\exp}(T_n)$ is the experimentally measured vapor pressure at temperature T_n. The minimization was carried out using the "Solver" feature in Microsoft Excel 2000 (9.0.6926 SP-3).

In cases when the primary data involved the sublimation vapor pressure ($p_{\mathrm{S}}^{\mathrm{o}}$), conversion to sub-cooled liquid vapor pressure ($p_{\mathrm{L}}^{\mathrm{o}}$) values proceeded using (Prausnitz, 1969):

$$p_{\mathrm{L}}^{\mathrm{o}}(\mathrm{atm}) = 10^{\gamma} \qquad 1.4$$

$$\gamma = \log_{10} p_{\mathrm{S}}^{\mathrm{o}} + \frac{\Delta \bar{H}_{\mathrm{fus}}}{2.30259\, R\, T_{\mathrm{mp}}} \left(\frac{T_{\mathrm{mp}} - T}{T} \right) \qquad 1.5$$

where T_{mp} (K) is the melting point, $\Delta \overline{H}_{\mathrm{fus}}$ (J mol^{-1}) is the molar heat of fusion at T_{mp}, and R (J mol^{-1} K^{-1}) is the gas constant.

1.1. Antoine coefficients for sub-cooled liquid-phase vapor pressures were derived from solid-phase vapor pressure data and $\Delta \overline{H}_{\mathrm{fus}}$ values measured by Verevkin (1998).

1.2. Antoine coefficients for sub-cooled liquid-phase vapor pressures were derived from solid-phase vapor pressure data measured by Aihara (1960). Values for $\Delta \overline{H}_{\mathrm{fus}}$ for these compounds were estimated using the method of Jain *et al.* (2004).

1.3. Antoine coefficients for sub-cooled liquid-phase vapor pressures were derived from solid-phase vapor pressure data and $\Delta \overline{H}_{\mathrm{fus}}$ values measured by Verevkin (1999).

1.4. Antoine coefficients for sub-cooled liquid-phase vapor pressures were derived from solid-phase vapor pressure data and $\Delta \overline{H}_{\mathrm{fus}}$ values measured by Rai and Mandal (1990).

1.5. Antoine coefficients for sub-cooled liquid-phase vapor pressures were derived from solid-phase vapor pressure data measured by Davies *et al*. (1959). Values for $\Delta \overline{H}_{\mathrm{fus}}$ for these compounds were estimated using the method of Jain *et al.* (2004).

1.6. Antoine coefficients were obtained from Lemmon *et al.* (2000).

1.7. Antoine coefficients were derived by fitting reduced-pressure boiling point data obtained from the Beilstein Crossfire Online Database – BS0303PR

(http://www.beilstein.com).

1.8. Antoine coefficients for sub-cooled liquid-phase vapor pressures were derived from solid-phase vapor pressure data and values for $\Delta\overline{H}_{fus}$ from Monte and Hillesheim (2001a).

1.9. Antoine coefficients were derived from liquid-phase vapor pressure data measured by Nelson and Wales (1925).

1.10. Antoine coefficients were derived from liquid-phase vapor pressure data measured by Hatton *et al*. (1962).

1.11. Antoine coefficients were derived from liquid-phase vapor pressure data measured by Katayama (1988).

1.12. Antoine coefficients for sub-cooled liquid-phase vapor pressures were derived from solid-phase vapor pressures measured by Roux *et al*. (1998). $\Delta\overline{H}_{fus}$ for dimethyl-benzene-1,3-dicarboxylate was obtained from Steele *et al*. (1997). $\Delta\overline{H}_{fus}$ for dimethyl-benzene-1,4-dicarboxylate was obtained from the Beilstein Crossfire Online Database – BS0303PR (http://www.beilstein.com).

1.13. Antoine coefficients were derived from vapor pressure data measured by Verevkin *et al*. (1998).

1.14. Antoine coefficients for sub-cooled liquid-phase vapor pressures were derived from solid-phase vapor pressure data and values for $\Delta\overline{H}_{fus}$ from Monte and Hillesheim (2001c).

1.15. Antoine coefficients were derived from solid-phase vapor pressure data measured by Colomina *et al*. (1985). Values of $\Delta\overline{H}_{fus}$ for these compounds were estimated using the method of Jain *et al.* (2004).

1.16. Antoine coefficients were derived from solid-phase vapor pressure data and $\Delta\overline{H}_{fus}$ values measured by Lee *et al*. (1997)

1.17. Antoine coefficients were derived from solid-phase vapor pressure data from Oja and Suuberg (1999). Values of $\Delta\overline{H}_{fus}$ for these compounds were obtained from Shafizadeh *et al*. (1970)

1.18. Antoine coefficients were derived from liquid-phase vapor pressure data from Vacek and Stanek (1959).

1.19. Antoine coefficients were derived from solid-phase vapor pressure data from Edwards (1950). Values of $\Delta\overline{H}_{fus}$ for these compounds were obtained from Lemmon *et al.* (2000).

1.20. Antoine coefficients were derived from solid-phase vapor pressure data from Ribeiro da Silva *et al*. (1992). Values of $\Delta\overline{H}_{fus}$ for these compounds were obtained from Lemmon *et al.* (2000).

1.21. Antoine coefficients were derived from solid-phase vapor pressure data and $\Delta\overline{H}_{fus}$ values measured by Monte and Hillesheim (2001b).

1.22. Antoine coefficients were derived from solid-phase vapor pressure data from Ribeiro da Silva *et al*. (1999). $\Delta\overline{H}_{fus}$ values for 2-nitrobenzoic acid, 3-nitrobenzoic acid, and 4-nitrobenzoic acid were obtained from da Silva *et al*. (1999). $\Delta\overline{H}_{fus}$ values for the methoxy nitrobenzoic acids were estimated using the method of Jain *et al.* (2004).

2. When utilized in this work, the coefficients are for the form of the Antoine parameterization described by Rohac *et al*. (1999):

$$\ln\left(p_{\mathrm{L}}^{\mathrm{o}}\right) = A - \left(\frac{B}{T+C}\right) \qquad (1.6)$$

for $p_{\mathrm{L}}^{\mathrm{o}}$ in kPa and T in Kelvin.

3. When utilized in this work, the form of the modified Clausius-Clapeyron equation is

$$p_{\mathrm{L}}^{\mathrm{o}}(\mathrm{atm}) = \exp\left\{\left(\frac{B}{RA}\right)\left[1.8\left(1-\frac{A}{T}\right)+0.8\ln\left(\frac{A}{T}\right)\right]\right\} \qquad (1.7)$$

(e.g., see Schwarzenbach *et al.*, 1993) where R (J mol^{-1} K^{-1}) is the gas constant, $B = \Delta\overline{H}_{\mathrm{vap}}$ (J mol^{-1}) is the molar heat of vaporization, and $A = T_{\mathrm{bp}}$ (K) is the boiling point at 1 atm of pressure.

3.1. Values of $A = T_{\mathrm{bp}}$ were taken from Brown and Stein (2000). Values of $B = \Delta\overline{H}_{\mathrm{vap}}$ were taken from Lemmon *et al.* (2000).

3.2. Values of $A = T_{\mathrm{bp}}$ were taken from Brown and Stein (2000). Values of $B = \Delta\overline{H}_{\mathrm{vap}}$ were derived by fitting reduced-pressure boiling point data taken from Beilstein Crossfire Online Database – BS0303PR (http://www.beilstein.com) to Eq.(1.7).

3.3. Values of $A = T_{\mathrm{bp}}$ taken from Beilstein Crossfire Online Database – BS0303PR (http://www.beilstein.com). Values of $B = \Delta\overline{H}_{\mathrm{vap}}$ were taken from Lemmon *et al.* (2000).

4. Clausius-Clapeyron parameterization in the form:

$$\log p_{\mathrm{L}}^{\mathrm{o}} = A - \frac{B}{T} \qquad (1.8)$$

4.1. Coefficients A and B provided by Schwarzenbach *et al*. (1988) for sub-cooled liquid vapor pressures with $p_{\mathrm{L}}^{\mathrm{o}}$ in units of atm.

4.2. Coefficients A and B provided by Egerton *et al*. (1951) with $p_{\mathrm{L}}^{\mathrm{o}}$ in units of Torr.

4.3. Coefficients A and B provided by Bruckmann and Willner (1983) with $p_{\mathrm{L}}^{\mathrm{o}}$ in units of Torr.

Table 1. Saturated and Aromatic Oxygenated Compounds in the SIMPOL.1 Basis and Test Sets Not Found in *Asher et al*. (2002) or *Asher and Pankow* (Asher and Pankow, 2006) and their Vapor Pressure Parameterizations.

Compound	**Formula**	T_{MIN} **(K)**	T_{MAX} **(K)**	**Method/ Source**	**Units for** p_L^o	***A***	***B***	***C***
2-ethyl-hexanoic acid	$C_8H_{16}O_2$	154.75	500.7	3.1	atm	500.7	75.6	NA[a]
4-hydroxybiphenyl	$C_{12}H_{10}O$	273.15	393.15	1.1	atm	4.70776383	3000.2367	-19.2077
2-hydroxybiphenyl	$C_{12}H_{10}O$	273.15	393.15	1.1	atm	5.54610878	3000.4302	-23.46
4-(phenylmethyl)-phenol	$C_{13}H_{12}O$	273.15	393.15	1.2	atm	5.07006745	3001.3786	-44.1157
2-methyl-4-(t-butyl)-phenol	$C_{11}H_{16}O$	273.15	393.15	1.2	atm	5.19868532	2999.7694	-9.04344
2,4,6-tri-(t-butyl)-phenol	$C_{18}H_{30}O$	273.15	393.15	1.2	atm	5.49062056	3000.1363	-17.0523
4-hydroxy-benzaldehyde	$C_7H_6O_2$	273.15	393.15	1.2	atm	5.02355003	3000.8096	-31.7091
1-(4-hydroxyphenyl)-ethanone	$C_8H_8O_2$	273.15	393.15	1.2	atm	4.96236776	3001.2275	-40.8163
4-(t-butyl)-phenol	$C_{10}H_{14}O$	273.15	393.15	1.3	atm	6.09100407	3000.2064	-18.6034
2-(t-butyl)-4-methylphenol	$C_{11}H_{16}O$	273.15	393.15	1.3	atm	5.82327537	2999.6694	-6.89021
5-methyl-2-(t-butyl)-phenol	$C_{11}H_{16}O$	273.15	393.15	1.3	atm	6.04871460	3000.0040	-14.1917
1-napthol	$C_{10}H_8O$	273.15	393.15	1.4	atm	5.47148128	3000.2975	-20.5635
2-napthol	$C_{10}H_8O$	273.15	393.15	1.4	atm	5.46967874	3000.6935	-29.2126

[a]NA = Not Applicable

Table 2. Amides in the SIMPOL.1 Basis and Test Sets and their Vapor Pressure Parameterizations.

Compound	Formula	T_{MIN} (K)	T_{MAX} (K)	Method/ Source	Units for p_L^o	*A*	*B*	*C*
octanamide	$C_8H_{17}NO$	325	374	1.5	atm	2.98625039	1791.9555	-100.1569
heptanamide	$C_7H_{15}NO$	345	366	1.5	atm	2.96863086	1796.5450	-88.72823
hexanamide	$C_6H_{13}NO$	338	368	1.5	atm	3.24706267	1789.6416	-86.06252
pentanamide	$C_5H_{11}NO$	333	374	1.5	atm	3.50524533	1788.1264	-80.58214
butyramide	C_4H_9NO	298	341	1.5	atm	3.79284235	1786.0878	-80.55015
formamide	CH_3NO	343	634	1.6	atm	7.5852	3881.305	27.655
propanamide	C_3H_7NO	318	346	1.5	atm	3.80708626	1785.642	-75.03003
acetamide	C_2H_5NO	298	349	1.5	atm	4.54802005	2003.6692	-69.76276
butyl-acetamide	$C_6H_{13}NO$	261	502	3.1	atm	502	76	NA[a]
n-methyl-butyramide	$C_5H_{11}NO$	352	429	1.7	atm	6.93228177	2711.3609	-77.11400
ethyl-formamide	C_3H_7NO	243	471	3.1	atm	471.2	58.44	NA
methyl-acetamide	C_3H_7NO	303	363	1.6	atm	-0.06922	144.114	-277.873
methyl-formamide	C_2H_5NO	268	456	3.1	atm	455.7	56.19	NA
n,n-dimethyl-cyclohexane-carboxamide	$C_9H_{17}NO$	312	393	1.7	atm	7.08562742	3403.4356	-10.87568
n,n-diethyl-butanamide	$C_8H_{17}NO$	308	479	1.7	atm	4.25473575	1732.7303	-75.49241
dimethyl-propanamide	$C_5H_{11}NO$	228	448	3.1	atm	447.7	52.89	NA
diethyl-formamide	$C_5H_{11}NO$	303	363	1.6	atm	5.06358	2046.3630	-35.77400
dimethyl-acetamide	C_4H_9NO	303	363	1.6	atm	6.09451	2725.9600	28.20900
dimethyl-formamide	C_3H_7NO	303	363	1.6	atm	3.93068	1337.7160	-82.65000
1-methyl-piperidin-2-one	$C_6H_{11}NO$	336	496	1.7	atm	4.11508797	1781.2912	-71.93089

[a]NA = Not Applicable

Table 3. Amines in the SIMPOL.1 Basis and Test Sets and their Vapor Pressure Parameterizations.

Compound	Formula	T_{MIN} (K)	T_{MAX} (K)	Method/ Source	Units for p_L^o	*A*	*B*	*C*
hexylamine	$C_6H_{15}N$	258	403	3.1	atm	403	45.13	NA[a]
1,2-ethane-diamine	$C_2H_8N_2$	300	391	1.6	atm	4.22368	1302.256	-81.788
1-pentylamine	$C_5H_{13}N$	218	375	3.1	atm	375	40.15	NA
1-butylamine	$C_4H_{11}N$	224	351	3.1	atm	351	35.84	NA
isobutylamine	$C_4H_{11}N$	223	342	1.6	atm	4.41304	1317.873	-42.421
2-butylamine	$C_4H_{11}N$	169	336	3.1	atm	336	32.64	NA
1-propylamine	C_3H_9N	296	351	1.6	atm	4.05136	1044.028	-62.314
tert-butylamine	$C_4H_{11}N$	292	348	1.6	atm	3.90694	992.719	-62.727
2-propylamine	C_3H_9N	277	334	1.6	atm	4.01507	985.65	-59.079
ethylamine	C_2H_7N	191	290	1.6	atm	4.45586	1121.445	-37.854
methylamine	CH_5N	190	267	1.6	atm	4.5199	1034.977	-37.574
dibutylamine	$C_8H_{19}N$	211	430	3.1	atm	430	49.47	NA
n-propyl-1-propanamine	$C_6H_{15}N$	210	383	3.1	atm	383	40.1	NA
dimethyl-hydroxylamine	C_2H_7NO	291	363	1.6	atm	4.67111	1405.452	-72.215
n-methyl-1-butanamine	$C_5H_{13}N$	198	364	3.1	atm	364.2	32.9	NA
n-(1-methylethyl)-2-propanamine	$C_6H_{15}N$	177	357	3.1	atm	357	34.72	NA
diethylamine	$C_4H_{11}N$	304	334	1.6	atm	2.86193	559.071	-132.974
isopropyl-methylamine	$C_4H_{11}N$	n.a.	325	3.1	atm	324.7	30.93	NA
dimethylamine	C_2H_7N	201	280	1.6	atm	4.29371	995.445	-47.869
triethylamine	$C_6H_{15}N$	323	367	1.6	atm	2.98368	695.814	-128.271
trimethylamine	C_3H_9N	193	277	1.6	atm	4.01613	970.297	-34.06
4-amino-3-methylbenzoic	$C_8H_9NO_2$	367	383	1.8	atm	7.46559491	4382.9157	-22.73268
3-amino-4-methylbenzoic	$C_8H_9NO_2$	363	377	1.8	atm	7.40280084	4382.5272	-11.12597
3-amino-2-methylbenzoic	$C_8H_9NO_2$	367	381	1.8	atm	4.20102715	2615.3446	-73.49192
2-amino-6-methylbenzoic	$C_8H_9NO_2$	339	355	1.8	atm	4.62093277	2614.7784	-73.65167
2-amino-5-methylbenzoic	$C_8H_9NO_2$	345	361	1.8	atm	4.56178158	2614.4038	-65.50829
2-amino-3-methylbenzoic	$C_8H_9NO_2$	343	343	1.8	atm	4.55909601	2614.2022	-61.23092
o-amino-toluene	C_7H_9N	252	473	3.1	atm	473	57.9	NA
1-amino-2,4-dimethylbenzene	$C_8H_{11}N$	325	485	1.6	atm	5.18072	2293.277	-41.261
1-amino-4-ethylbenzene	$C_8H_{11}N$	325	491	1.6	atm	5.07568	2318.392	-33.508
1-amino-2,6-dimethylbenzene	$C_8H_{11}N$	317	491	1.6	atm	4.70051	2157.756	-32.151
m-amino-toluene	C_7H_9N	241	476	3.1	atm	476	45.6	NA
p-amino-toluene	C_7H_9N	315	473	3.1	atm	4.71884	1961.716	-57
n-ethyl-*n*-phenylamine	$C_8H_{11}N$	323	480	1.6	atm	5.64275	2809.017	20.856
n-methyl-phenylamine	C_7H_9N	323	473	1.9	atm	4.99409	2226.576	-22.456
n,n-dimethyl-n-phenyl-amine	$C_8H_{11}N$	302	466	1.6	atm	4.83003	2117.236	-27.606
phenylamine	C_6H_7N	304	457	1.10	atm	4.34541	1661.858	-74.048
methyl-*n*-phenyl-amine	C_7H_9N	302	458	1.6	atm	4.8271	2003.528	-41.973
1-(diethylamino)-2-propanone	$C_7H_{15}NO$	311	432	1.7	atm	4.75094205	1893.0129	-33.68959
1-(dimethylamino)-2-propanone	$C_5H_{11}NO$	300	399	1.7	atm	1.74075706	325.94917	-208.9975
triethanolamine	$C_6H_{15}NO_3$	290	390	1.7	atm	7.93043866	4389.6929	-30.89348

[a]NA = Not Applicable

Table 4. Esters in the SIMPOL.1 Basis and Test Sets and their Vapor Pressure Parameterizations.

Compound	Formula	T_{MIN} (K)	T_{MAX} (K)	Method/ Source	Units for p_L^o	*A*	*B*	*C*
n-butyl-benzoate	$C_{11}H_{14}O_2$	374	474	1.11	atm	5.574224	2552.706	-49.4701
2-methyl-propyl-benzoate	$C_{11}H_{14}O_2$	370	467	1.11	atm	5.24134	2550.831	-22.973
ethyl-2-butoxy-ethanoate	$C_8H_{16}O_3$	210	465	3.1	atm	465.2	59.54	NA[a]
n-propyl-benzoate	$C_{10}H_{12}O_2$	359	458	1.11	atm	4.71837	2185.719	-39.467
phenyl-methyl-ethanoate	$C_9H_{10}O_2$	319	429	1.6	atm	2.34301	791.918	-175.864
ethyl-benzoate	$C_8H_8O_2$	239	485	3.1	atm	485	45.19	NA
methyl-benzoate	$C_8H_8O_2$	333	438	1.11	atm	3.701407	1354.186	-108.104
acetic-acid,-phenyl-ester	$C_8H_8O_2$	311	469	1.6	atm	5.02585	2174.699	-36.045
methyl-heptanoate	$C_8H_{16}O_2$	323	447	1.7	atm	4.178764	1449.989	-98.7947
hexyl-ethanoate	$C_8H_{16}O_2$	330	445	1.7	atm	4.086754	1449.005	-88.9979
ethyl-hexanoate	$C_8H_{16}O_2$	298	441	1.7	atm	4.058232	1448.492	-83.9931
1-methyl-propyl-butanoate	$C_8H_{16}O_2$	273	424	3.1	atm	424.65	47	NA
propyl-pentanoate	$C_8H_{16}O_2$	202	441	3.1	atm	440.7	40	NA
ethyl-4-methyl-pentanoate	$C_8H_{16}O_2$	284	433	1.6	atm	4.69631	1847.593	-40.092
1-methyl-ethyl-pentanoate	$C_8H_{16}O_2$	324	438	3.2	atm	438.05	38.5	NA
propyl-3-methyl-butanoate	$C_8H_{16}O_2$	281	429	1.6	atm	4.7678	1873.942	-35.977
2-methyl-propyl-butanoate	$C_8H_{16}O_2$	277	430	1.6	atm	4.75676	1927.291	-25.089
2-methyl-propyl-2-methyl-propanoate	$C_8H_{16}O_2$	277	421	1.6	atm	4.76033	1806.356	-40.698
methyl-pentanoate	$C_6H_{12}O_2$	273	410	3.1	atm	410	43.1	NA
ethyl-butanoate	$C_6H_{12}O_2$	255	394	1.6	atm	4.33187	1509.443	-45.284
methyl-3-methyl-butanoate	$C_6H_{12}O_2$	254	390	1.6	atm	4.52819	1582.466	-40.123
2-methyl-propyl-ethanoate	$C_6H_{12}O_2$	252	391	1.6	atm	4.53676	1625.875	-32.494
ethyl-2-methyl-propanoate	$C_6H_{12}O_2$	249	383	1.6	atm	4.48202	1536.985	-39.904
dimethyl-1,2-benzenedicarboxylate	$C_{10}H_{10}O_4$	324	552	2	kPa	14.82359	4660.937	-99.10860
dimethyl-benzene-1,3-dicarboxylate	$C_{10}H_{10}O_4$	294	309	1.12	atm	3.370812	1795.995	-93.4013
dimethyl-benzene-1,4-dicarboxylate	$C_{10}H_{10}O_4$	311	330	1.12	atm	6.465142	3374.277	-13.1114
dimethyl-cyclohexane-1,3-dicarboxylate	$C_{10}H_{16}O_4$	357	551	1.7	atm	4.01033	1813.998	-94.748
diethyl-hexanedicarboxylate	$C_{10}H_{18}O_4$	350	524	1.6	atm	5.26245	2572.141	-34.746
di-n-butyl-ethanedicarboxylate	$C_{10}H_{18}O_4$	356	513	3.2	atm	513	52	NA
diethyl-cyclopentane-1,1-dicarboxylate	$C_{11}H_{18}O_4$	293	323	1.13	atm	0.365182	531.396	-187.068
diethyl-cyclopropane-1,1-dicarboxylate	$C_9H_{14}O_4$	288	318	1.13	atm	0.602863	530.6848	-181.491
diethyl-ethanedicarboxylate	$C_6H_{10}O_4$	320	459	1.6	atm	5.98158	2537.141	-34.06
1,2-ethanediol-diacetate	$C_6H_{10}O_4$	336	466	1.7	atm	6.36566	2933.612	0.0328626
dimethyl-propanedicarboxylate	$C_5H_8O_4$	308	454	1.6	atm	5.22732	2143.666	-43.448
diethyl-cyclobutane-1,1-dicarboxylate	$C_{10}H_{16}O_4$	288	318	1.13	atm	0.471713	530.8136	-183.234
ethyl-cyclopentanecarboxylate	$C_9H_{14}O_4$	274	308	1.13	atm	0.862263	470.0863	-168.379
ethyl-cyclobutanecarboxylate	$C_8H_{12}O_4$	273	308	1.13	atm	0.975704	448.3845	-162.792
methyl-cyclobutanecarboxylate	$C_7H_{10}O_4$	268	323	1.13	atm	0.626052	282.3435	-188.782
ethyl-cyclopropanecarboxylate	$C_7H_{10}O_4$	278	308	1.13	atm	1.622442	510.881	-154.414
methyl-cyclopropanecarboxylate	$C_6H_8O_4$	273	313	1.13	atm	1.60185	434.8424	-162.377
ethyl-2-propoxyethanoate	$C_7H_{14}O_3$	273	452	3.1	atm	452	55.62	NA
methyl-dimethoxyethanoate	$C_5H_{10}O_4$	325	344	1.7	atm	1.957257	479.2967	-206.293

[a]NA = Not Applicable

Table 5. Ethers in the SIMPOL.1 Basis and Test Sets and their Vapor Pressure Parameterizations.

Compound	Formula	T_{MIN} (K)	T_{MAX} (K)	Method/ Source	Units for p_L^o	*A*	*B*	*C*
diethyl ether	$C_4H_{10}O$	250	329	1.6	atm	4.022	1062.64	-44.93
1-butoxy-2-ethoxyethane	$C_8H_{18}O_2$	273	435	3.1	atm	435	50.94	NA[a]
1,2-dipropoxyethane	$C_8H_{18}O_2$	273	435	3.1	atm	435	50.62	NA
1-(2-methoxyethoxy)-butane	$C_7H_{16}O_2$	273	420	3.1	atm	420	47.83	NA
1,3-diethoxypropane	$C_7H_{16}O_2$	273	414	3.1	atm	413.7	45.92	NA
1,2-epoxy-3-isopropoxy-propane	$C_6H_{12}O_2$	273	405	3.1	atm	404.7	43.5	NA
1,1-dimethoxybutane	$C_6H_{14}O_2$	273	387	3.1	atm	387	41.7	NA
dimethoxy-methane	$C_3H_8O_2$	273	308	1.6	atm	4.029975	1068.35	-50.409
2-*n*-butoxy-1-ethanol	$C_6H_{14}O_2$	299	443	1.6	atm	4.25626	1511.414	-88.815
2-(2-methylpropoxy)-ethanol	$C_6H_{14}O_2$	344	432	1.6	atm	4.73287	1766.888	-59.128
2-(2-methoxyethoxy)-tetrahydro-2H-pyran	$C_8H_{16}O_3$	273	471	3.1	atm	471.3	60	NA
2-methoxy-tetrahydro-pyran	$C_6H_{12}O_2$	273	401	3.1	atm	401.7	42.7	NA
2-phenyl-1,3-dioxolane	$C_9H_{10}O_2$	273	413	3.1	atm	413	62.13	NA
1,3-dioxacyclooctane	$C_6H_{12}O_2$	273	407	3.1	atm	407	44.8	NA
5,5-dimethyl-1,3-dioxane	$C_6H_{12}O_2$	273	398	3.1	atm	398	41	NA
4,4-dimethyl-1,3-dioxane	$C_6H_{12}O_2$	299	406	1.6	atm	4.69235	1805.43	-21.161
1,3-dioxepan	$C_5H_{10}O_2$	195	392	3.1	atm	392	41.293	NA
cis-2,4-dimethyl-1,3-dioxane	$C_6H_{12}O_2$	273	391	3.1	atm	390.65	40	NA
trans-2,2,4,6-tetramethyl-1,3-dioxane	$C_8H_{16}O_2$	273	385	3.1	atm	384.65	41.9	NA
4-methyl-1,3-dioxane	$C_5H_{10}O_2$	273	387	3.1	atm	387.2	39	NA
1,3-dioxane	$C_4H_8O_2$	230	378	3.1	atm	378.7	39.09	NA
1,4-dioxane	$C_4H_8O_2$	293	374	1.6	atm	4.58135	1570.093	-31.297
1,3-dioxolan	$C_3H_6O_2$	280	355	1.6	atm	4.11859	1237.377	-48.735
1,1-dimethoxy-2-butene	$C_6H_{12}O_2$	273	399	3.3	atm	399	43.26	NA
1,1-dimethoxy-ethene	$C_4H_8O_2$	273	362	3.3	atm	362	35.4	NA
3-(3,4-dimethoxyphenyl)-propanoic acid	$C_{11}H_{14}O_4$	352	366	1.14	atm	7.756857	4306.957	-38.27643
3,4-dimethoxybenzoicacid	$C_9H_{10}O_4$	355	379	1.15	atm	2.097138	1788.771	-128.2405
3,5-dimethoxybenzoicacid	$C_9H_{10}O_4$	359	378	1.15	atm	6.221483	3502.410	-60.2279
2,6-dimethoxybenzoicacid	$C_9H_{10}O_4$	355	378	1.15	atm	5.065479	3089.971	-67.7979
3-(4-methoxyphenyl)-propanoic acid	$C_{10}H_{12}O_3$	341	357	1.14	atm	7.941833	4306.262	-17.41505
3-(2-methoxyphenyl)-propanoic acid	$C_{10}H_{12}O_3$	331	347	1.14	atm	4.844668	2614.925	-78.08624
4-methoxy-benzaldehyde	$C_8H_8O_2$	283	522	1.7	atm	5.395640	2712.836	-19.35678
4-methoxy-phenol	$C_7H_8O_2$			1.16	atm	7.871883	3998.240	13.38746
(phenoxymethyl)-oxirane	$C_9H_{10}O_2$	276	518	3.1	atm	518.2	69.85	NA
2,4-dimethoxybenzoic-acid	$C_9H_{10}O_4$	346	367	1.15	atm	2.168045	1798.434	-126.5433
2,3-dimethoxybenzoic-acid	$C_9H_{10}O_4$	336	356	1.15	atm	2.771580	1789.141	-121.5258
levoglucosan	$C_6H_{10}O_5$	344	386	1.17	atm	11.21204	6218.366	0.277922

[a]NA = Not Applicable

Table 6. Nitrates in the SIMPOL.1 Basis and Test Sets and their Vapor Pressure Parameterizations.

Compound	Formula	T_{MIN} (K)	T_{MAX} (K)	Method/ Source	Units for p_L^o	*A*	*B*	*C*
phenylmethyl-nitrate	$C_7H_7NO_3$	315	393	1.7	atm	6.06887	2756.749	-23.1218
3-methylbutyl-nitrate	$C_5H_{11}NO_3$	278	421	1.6	atm	4.74613	1785.807	-43.975
butyl-nitrate	$C_4H_9NO_3$	273	343	1.6	atm	5.46933	2177.065	-4.855
2-methylpropyl-nitrate	$C_4H_9NO_3$	273	343	1.6	atm	5.32531	2045.425	-8.996
propylnitrate	$C_3H_7NO_3$	273	343	1.6	atm	4.86209	1721.723	-27.66
1-methylethyl-nitrate	$C_3H_7NO_3$	273	343	1.6	atm	3.54496	1018.568	-89.622
ethyl-nitrate	$C_2H_5NO_3$	273	333	1.6	atm	4.28523	1337.035	-48.37
cyclohexane-nitrate	$C_6H_{11}NO_3$	310	454	1.7	atm	6.04373	2754.808	6.99462
cyclopental-nitrate	$C_5H_9NO_3$	325	434	1.7	atm	6.46142	2755.340	-2.42039
2-nitro-2-[(nitrooxy)methyl]-1,3-propanediol-dinitrate	$C_4H_6N_4O_{11}$	313	353	1.18	atm	2.91814	3003.350	-34.1217
1,2,3-propanetrinitrate	$C_3H_5N_3O_9$	293	453	1.7	atm	5.95578	2759.095	-71.7407
2,2'-oxybis-ethanol-dinitrate	$C_4H_8N_2O_7$	288	333	1.18	atm	10.6353	4356.373	-19.4235

Table 7. Nitro-Containing Compounds in the SIMPOL.1 Basis and Test Sets and their Vapor Pressure Parameterizations.

Compound	Formula	T_{MIN} (K)	T_{MAX} (K)	Method/ Source	Units for p_L^o	*A*	*B*	*C*
2,4,6-trinitrotoluene	$C_7H_5N_3O_6$	323	423	1.19	atm	4.56962	2614.284	-83.151
1-nitrobutane	$C_4H_9NO_2$	191	426	3.1	atm	426.2	48.58	NA[a]
2-nitrobutane	$C_4H_9NO_2$	309	413	1.7	atm	4.69216	1838.834	-20.909
3-nitro-1-propanol	$C_3H_7NO_3$	345	412	1.7	atm	8.80410	4160.880	-0.131540
3-nitro-2-pentanol	$C_5H_{11}O_3$	333	403	1.7	atm	5.51023	1848.341	-122.252
3-nitro-2-butanol	$C_4H_9NO_3$	323	386	1.7	atm	5.69227	1848.229	-120.281
nitro-ethanol	$C_2H_5NO_3$	288	471	1.7	atm	25.58636	34204.889	869.171
2-nitro-1-propanol	$C_3H_7NO_3$	330	394	1.7	atm	7.306781	3511.292	9.79585
methyl-4-nitrobutanoate	$C_5H_9NO_4$	341	384	1.7	atm	12.2996	5419.999	-0.218889
ethyl-nitroacetate	$C_4H_7NO_4$	315	398	1.7	atm	0.41394	287.696	-240.865
ethyl-2-nitropropionate	$C_5H_9NO_4$	311	465	1.7	atm	3.56211	1154.632	-147.464
methyl-2-nitro-propionate	$C_4H_7NO_4$	326	376	1.7	atm	3.108	1024.515	-153.901
methyl-nitroacetate	$C_3H_5NO_4$	319	385	1.7	atm	1.81464	593.693	-197.577
1-nitromethyl-1-cyclohexanol	$C_7H_{13}NO_3$	343	404	1.7	atm	15.7061	6953.604	-0.19179
3-nitro-2-butanone	$C_4H_7NO_3$	329	365	1.7	atm	8.374270	3617.072	-0.060774
3-nitrophenol	$C_6H_5NO_3$	316	330	1.20	atm	5.039574	2613.383	-62.1157
4-nitrophenol	$C_6H_5NO_3$	328	353	4.1	atm	8.305	4180	NA
4-(1-methylpropyl)-2-nitrophenol	$C_{10}H_{13}NO_3$	328	353	4.1	atm	7.59	3752	NA
5-methyl-2-nitrophenol	$C_7H_7NO_3$	328	353	4.1	atm	6.412	3120	NA
4-methyl-2-nitrophenol	$C_7H_7NO_3$	328	353	4.1	atm	6.392	3105	NA
3-methyl-2-nitrophenol	$C_7H_7NO_3$	328	353	4.1	atm	6.315	3063	NA
2-nitrophenol	$C_6H_5NO_3$	328	353	4.1	atm	5.735	2776	NA
5-methyl-2-nitrobenzoic acid	$C_8H_7NO_4$	355	371	1.21	atm	4.17166	2616.891	-81.851
2-methyl-6-nitrobenzoic acid	$C_8H_7NO_4$	355	369	1.21	atm	7.518180	4286.549	-15.02470
4-methyl-3-nitrobenzoic acid	$C_8H_7NO_4$	315	377	1.21	atm	4.16965	2615.35	-74.397
2-nitrobenzoic acid	$C_7H_5NO_4$	346	366	1.22	atm	4.33022	2615.098	-74.412
3-nitrobenzoic acid	$C_7H_5NO_4$	347	361	1.22	atm	4.32231	2615.301	-73.178
3-methyl-2-nitrobenzoic acid	$C_8H_7NO_4$	371	385	1.21	atm	4.202501	2614.432	-69.2644
3-methyl-4-nitrobenzoic acid	$C_8H_7NO_4$	315	379	1.21	atm	4.239659	2614.377	-67.9823
2-methyl-3-nitrobenzoic acid	$C_8H_7NO_4$	357	371	1.21	atm	4.39919	2613.748	-70.334
4-nitrobenzoic acid	$C_7H_5NO_4$	367	381	1.22	atm	4.32001	2616.016	-61.137
6-methyl-2,4-dinitrophenol	$C_7H_6N_2O_5$	328	353	4.1	atm	7.929	3970	NA
2,4-dinitrophenol	$C_6H_4N_2O_5$	328	353	4.1	atm	7.392	3680	NA
2,5-dinitrophenol	$C_6H_4N_2O_5$	328	353	4.1	atm	7.229	3580	NA
4-formyl-2-nitrophenol	$C_7H_5NO_4$	328	353	4.1	atm	7.258	3540	NA
4-methoxy-2-nitrophenol	$C_7H_7NO_4$	328	353	4.1	atm	5.518	2673	NA
3-methoxy-2-nitrobenzoic acid	$C_8H_7NO_5$	398	410	1.22	atm	3.29532	2619.381	-98.678
4-methoxy-3-nitrobenzoic acid	$C_8H_7NO_5$	387	401	1.22	atm	3.48938	2616.311	-92.307
3-methoxy-4-nitrobenzoic acid	$C_8H_7NO_5$	388	402	1.22	atm	3.63341	2617.414	-89.609

[a]NA = Not Applicable

Table 8. Hydroperoxides, Peroxides, Hydroperoxy Acids, and Peroxycarbonyls in the SIMPOL.1 Basis and Test Sets and their Vapor Pressure Parameterizations.

Compound	Formula	T_{MIN} (K)	T_{MAX} (K)	Method/ Source	Units for p_L^o	*A*	*B*	*C*
di-n-butyl-peroxide	$C_8H_{18}O_2$	328	353	1.7	atm	1.77561	1139.512	-0.019256
di-(1-methyl-propyl)-peroxide	$C_8H_{18}O_2$	316	332	1.7	atm	7.295134	2840.558	-0.105291
di-*tert*-butyl-peroxide	$C_8H_{18}O_2$	253	373	4.2	Torr	7.14	-1621	NA[a]
diethyl-peroxide	$C_4H_{10}O_2$	253	333	4.2	Torr	7.356	-1517	NA
1-methyl-1-phenylethyl-hydroperoxide	$C_9H_{12}O_2$	316	390	1.7	atm	4.06825	1032.085	-201.3547
tert-butyl-hydroperoxide	$C_4H_{10}O_2$	273	393	4.2	Torr	8.891	-2432	NA
ethylhydroperoxide	$C_2H_6O_2$	253	363	4.2	Torr	8.834	-2228	NA
methylhydroperoxide	CH_4O_2	253	313	4.2	Torr	8.38	-1972	NA
butyryl-hydroperoxide	$C_4H_8O_3$	273	393	4.2	Torr	8.83	-2376	NA
propionylhydroperoxide	$C_3H_6O_3$	273	393	4.2	Torr	8.623	-2256	NA
acetyl-hydroperoxide	$C_2H_4O_3$	273	383	4.2	Torr	8.911	-2311	NA
peroxyacetylnitrate	$C_2H_3O_4N$	223	291	4.3	Torr	8.1474	-1992.1	NA

[a]NA = Not Applicable

References

Aihara, A. (1960) Estimation of the energy of hydrogen bonds formed in crystals. II. Phenols. *Bulletin of the Chemical Society of Japan* **33**, 194-200.

Asher, W.E., Erdakos, G.B., Seinfeld, J.H., Pankow, J.F. (2002) Estimating the vapor pressures of multi-functional oxygen-containing organic compounds using group contribution methods. *Atmospheric Environment* **36**, 1483-1498.

Asher, W.E., Pankow, J.F. (2006) Vapor pressure prediction for alkenoic and aromatic organic compounds by a UNIFAC-based group contribution method. *Atmospheric Environment* **40**, 3588-3600.

Brown, R.L., Stein, S.E. (2000) Boiling Point Data. In: W.G. Mallard and P.J. Linstrom (Eds.) NIST Chemistry WebBook, NIST Standard Reference Database Number 69, February 2000, National Institute of Standards and Technology, Gaithersburg (http://webbook.nist.gov).

Bruckmann, P.W., Willner, H. (1983) Infrared spectroscopic study of peroxyacetyl nitrate (PAN) and its decomposition products. *Environmental Science and Technology* **17**, 352-357.

Colomina, M., Jimenez, P., Roux, M.V., Turrion, C. (1985) Thermochemical properties of benzoic acid derivatives. XII. Vapor pressures and enthalpies of sublimation and formation of five dimethoxybenzoic acids. *J. Chemical Thermodynamics* **17**, 1091-1096.

Davies, M., Jones, A.H., Thomas, G.H. (1959) The lattice energies of the straight-chain primary amides. *Trans. Faraday Soc.* **55**, 1100-1108.

Edwards, G. (1950) The vapour pressure of 2,4,6-trinitrotoluene. *Trans. Faraday Soc.* **46**, 423-427.

Egerton, A.C., Emte, W., Minkoff, G.J. (1951) Some properties of organic peroxides. *Faraday Discuss. Chem. Soc.* **278**, 278-282.

Hatton, W.E., Hildenbrand, D.L., Sinke, G.C., Stull, D.R. (1962) Chemical thermodynamic properties of aniline. *J. Chemical and Engineering Data* **7**, 229-231.

Jain, A., Yang, G., Yalkowsky, S.H. (2004) Estimation of total entropy of melting of organic compounds. *Industrial and Engineering Chemistry Research* **43**, 4376-4379.

Katayama, H. (1988) Vapor pressures of methyl, ethyl, n-propyl, isobutyl, and n-butyl benzoates at reduced pressures, *J. Chemical and Engineering Data* **33**, 75-77.

Lee, M.-J., Change, Y.-K., Liu, H.-M., Chen, C.-H. (1997) *J. Chemical and Engineering Data* **42**, 349-352.

Lemmon, E.W., McLinden, M.O., Friend, D.G. (2000) Thermophysical Properties of Fluid Systems. In: W.G. Mallard and P.J. Linstrom (Eds.) NIST Chemistry WebBook, NIST Standard Reference Database Number 69, February 2000, National Institute of Standards and Technology, Gaithersburg (http://webbook.nist.gov).

Monte, M.J.S., Hillesheim, D.M. (2001a) Thermodynamic study of the sublimation of six aminomethylbenzoic acids. *J. Chemical Thermodynamics* **33**, 745-754.

Monte, M.J.S., Hillesheim, D.M. (2001b) Thermodynamic study of the sublimation of six methylnitrobenzoic acids, *J. Chemical Thermodynamics* **33**, 103-112.

Monte, M.J.S., Hillesheim, D.M. (2001c) Thermodynamic study on the sublimation of 3-phenylpropionic acid and of three methoxy substituted 3-phenylpropionic acids. *J. Chemical Thermodynamics* **33**, 837-847.

Nelson, O.A., Wales, H. (1925) Vapor pressures and boiling points of mono- and dimethylanilines and mono- and diethylanilines. *J. American Chemical Soc.* **47**, 867-872.

Oja, V., Suuberg, E.M. (1999) Vapor pressures and enthalpies of sublimation of d-glucose, d-xylose, cellobiose, and levoglucosan. *J. Chemical and Engineering Data* **44**, 26-29.

Prausnitz, J.M. (1969) *Molecular Thermodynamics of Fluid-Phase Equilibria*, Prentice-Hall, Englewoods Cliffs, NJ, USA. 523 pp.

Rai, U.S., Mandal, K.D. (1990) Some physicochemical studies on organic eutectics and 1:2 addition compounds. *Molecular Crystals and Liquid Crystals* **182B**, 387-404.

Reid, R.C., Prausnitz, J.M., Poling, B.E. (1987) *The Properties of Gases and Liquids*, 4th ed,

McGraw-Hill, New York, NY, USA. 741 pp.

Ribeiro da Silva, M.A.V. *et al.* (1999) Enthalpies of combustion, vapour pressures, and enthalpies of sublimation of three methoxynitrobenzoic acids. Vapour pressures and enthalpies of sublimation of the three nitrobenzoic acids. *J. Chemical Thermodynamics* **31**, 1429-1441.

Ribeiro da Silva, M.A.V., Reis, A.M.M.V., Monte, M.J.S., Bartolo, M.M.S.S.F., Rodrigues, J.A.R.G.O. (1992) Enthalpy of combustion, vapour pressures, and enthalpy of sublimation of 3-nitrophenol. *J. Chemical Thermodynamics* **24**, 653-659.

Rohac, V., Musgrove, J.E., Ruzicka, K., Ruzicka, V., Zabransky, M. (1999) Thermodynamic properties of dimethyl phthalate along the (vapour + liquid) saturation curve. *J. Chemical Thermodynamics* **31**, 971-986.

Roux, M.V. *et al.* (1998) Enthalpies of formation of methyl benzenecarboxylates, *J. Chem. Soc., Faraday Transactions* **94**, 887-890.

Schwarzenbach, R.P., Stierli, R., Folsom, B.R. Zeyer, J. (1988) Compound properties relevant for assessing the environmental partitioning of nitrophenols *Environmental Science and Technology* **22**, 83-92.

Shafizadeh, F., McGinnis, G.D., Philpot, C.W., Susott, R.A. (1970) Solid-state transition of 1,6-anhydro-b-d-glucopyranose. *Carbohydrate Research* **13**, 184-186.

Steele, W.V., Chirico, R.D., Knipmeyer, S.E. Nguyen, A. (1997) Vapor pressure, heat capacity, and density along the saturation line, measurements for dimethyl isophthalate, dimethyl carbonate, 1,3,5-triethylbenzene, pentafluorophenol, 4-tert-butylcatechol, r-methylstyrene, and N,N'-bis(2-hydroxyethyl)ethylenediamine, *J. Chemical and Engineering Data* **42**, 1008-1020.

Vacek, J., Stanek, J. (1959) Vapor pressures of some organic nitrates. *Chemicky Prumysl* **9**, 286-288.

Verevkin, S.P. (1998) Thermochemistry of phenols: experimental standard molar enthalpies of formation of 2-phenylphenol, 4-phenylphenol, 2,6-diphenylphenol, and 2,2'- and 4,4'-dihydroxybiphenyl, *J. Chemical Thermodynamics* **30**, 389-396.

Verevkin, S.P. (1999) Thermochemistry of phenols: quantification of the ortho-, para-, and meta-interactions in tert-alkyl substituted phenols. *J. Chemical Thermodynamics* **31**, 559-585.

Verevkin, S.P., Kümmerlina, M., Beckhaus, H.-D., Galli, C., Rüchardt, C. (1998) Do alkoxycarbonyl substituents stabilize small cycloalkane rings? European *J. Organic Chemistry* **1998**, 579-584.