JOURNAL OF PHYSICAL ORGANIC CHEMISTRY
J. Phys. Org. Chem. **12**, 675–680 (1999)

Solubility of gases and vapours in propan-1-ol at 298 K

Michael H. Abraham,[1]* Joelle Le,[1] William E. Acree, Jr[2] and Peter W. Carr[3]

[1]Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, UK
[2]Department of Chemistry, University of North Texas, Denton, Texas 76203-0068, USA
[3]Department of Chemistry, University of Minnesota, 207 Pleasant Street S.E., Minnepolis, Minnesota 55455, USA

Received 11 January 1999; revised 30 March 1999; accepted 15 April 1999

ABSTRACT: Literature values of the Ostwald solubility coefficient of gases and vapours in propan-1-ol at 298 K were combined with additional values calculated from solubilities in propan-1-ol and vapour pressures to yield a total of 79 $\log L^{\mathrm{PrOH}}$ values at 298 K. Seventy-seven of these values were correlated through the general solvation equation to give the regression

$$\log L^{\mathrm{PrOH}} = -0.028 - 0.185R_2 + 0.648\pi_2{}^{\mathrm{H}} + 4.022\Sigma\alpha_2{}^{\mathrm{H}} + 1.043\Sigma\beta_2{}^{\mathrm{H}} + 0.869\log \mathrm{L}^{16}$$
$$n = 77, r^2 = 0.9976, \mathrm{SD} = 0.12, F = 6073$$

A correlation equation was also constructed for the transfer of solutes from water to propan-1-ol. Both equations suggest that propan-1-ol as a solvent is less dipolar, more acidic and less basic than methanol or ethanol, but the differences between the three alcohols are very small. Comparison with equations for transfer to wet alcohols shows that the addition of water to alcohols has little effect on their dipolarity/polarizability or hydrogen bond basicity, but considerably increases the hydrogen bond acidity. The wet alcohols are more hydrophilic (less hydrophobic) than the dry alcohols. Copyright © 1999 John Wiley & Sons, Ltd.

KEYWORDS: propan-1-ol; hydrogen bond acidity; hydrogen bond basicity; solubility

INTRODUCTION

We have recently shown that the solubilities of gases and vapours in water,[1] methanol[2] and ethanol[3] can be correlated through the general solvation equation

$$\log SP = c + rR_2 + s\pi_2{}^{\mathrm{H}} + a\Sigma\alpha_2{}^{\mathrm{H}} + b\Sigma\beta_2{}^{\mathrm{H}} + l\log L^{16} \qquad (1)$$

where SP in the dependent variable is a property of a series of solutes in a given system and the independent variables are solute descriptors as follows:[4] R_2 is excess molar refraction, $\pi_2{}^{\mathrm{H}}$ the dipolarity/polarizability, $\sum\alpha_2{}^{\mathrm{H}}$ the overall or summation hydrogen bond acidity and $\sum\beta_2{}^{\mathrm{H}}$ the overall or summation hydrogen bond basicity. In the final descriptor, L^{16} is the Ostwald solubility coefficient on hexadecane at 298 K,[5] defined as

$$L = \frac{\text{concentration of solute in solution/}}{\text{concentration of solute in the gas phase}} \qquad (2)$$

The coefficients in Eqn. (1) are of considerable interest, as they refer to properties of the solvent phase. In particular, *s* will reflect the phase dipolarity/polarizability, *a* will be proportional to the solvent hydrogen bond basicity (since solutes that are acidic will interact with solvents that are themselves basic) and *b* will be proportional to the solvent hydrogen bond acidity; *l* is the resultant of two effects, (i) the work of creating a cavity in the solvent and (ii) general dispersion interactions between the solute and solvent. The former is an endoergic effect leading to a negative *l* coefficient, and the latter is an exothermic effect leading to a positive *l* coefficient. For all non-aqueous solvents the general dispersion effect predominates, and so *l* is positive. The magnitude of *l* can be taken as a measure of the solvent lipophilicity/hydrophobicity.

When Eqn. (1) was applied to log *L* values in methanol and ethanol,[2,3] the regression coefficients suggested that these alcohols are just as basic as water (in a hydrogen bond sense) but that they are much weaker hydrogen bond acids. Indeed, the two alcohols were slightly weaker hydrogen bond acids than chloroform,[6] as can be seen by the regression coefficients in Table 1. These conclusions from Eqn. (1) were not in agreement with solvatochromic studies on water and the alcohols, and so it seemed useful to extend the scope of Eqn. (1) to other alcohols for which there were enough data. In addition, any method for the prediction of gas–propan-1-ol partition coefficients,

---

**Correspondence to:* Michael H. Abraham, Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, UK.

Copyright © 1999 John Wiley & Sons, Ltd.

Table 1. Coefficients in Eqn. (1) for gas–solvent partitions

Solvent	*c*	*r*	*s*	*a*	*b*	*l*
Water	−1.271	0.822	2.743	3.904	4.814	−0.213
Methanol	−0.004	−0.215	1.173	3.701	1.432	0.769
Ethanol	0.012	−0.206	0.789	3.635	1.311	0.853
Propan-1-ol	−0.028	−0.185	0.648	4.022	1.043	0.869
Chloroform	0.168	−0.595	1.256	0.280	1.370	0.981
Hexadecane	0	0	0	0	0	1

L^{PrOH}, would be of interest in chemical engineering. A survey of the literature showed that there were enough data on propan-1-ol as a solvent to set up a statistically significant regression equation, and that is the main purpose of this paper. A second aim was to combine the log L^{PrOH} values with corresponding log L^{W} values for water solvent, through the equation

$$\log P^{PrOH/W} = \log L^{PrOH} - \log L^{W} \qquad (3)$$

and so to obtain values of log $P^{PrOH/W}$ for the transfer of solutes from water to propan-1-ol. These log $P^{PrOH/W}$ values can then be correlated through the alternative solvation equation

$$\log SP = c + rR_2 + s\pi_2{}^{H} + a\Sigma\alpha_2{}^{H} + b\Sigma\beta_2{}^{H} + \nu Vx \qquad (4)$$

where the final descriptor is the McGowan volume[7] in units of (cm^3 mol^{-1})/100.

The coefficients in Eqn. (4) again relate to the solvent properties, this time relative to those for water, and so will provide another set of data on propan-1-ol. Just like the *l* coefficient in Eqn. (1), the ν coefficient is also the resultant of (i) the cavity and (ii) the general dispersion interaction effects, but now relative to these effects in water. For all water–solvent systems we have studied, the ν coefficient is positive, owing to both a greater cavity effect in water and a larger general dispersion effect in the solvent. The magnitude of the ν coefficient can be taken as a measure of the solvent hydrophobicity.

RESULTS AND DISCUSSION

Values of log L^{PrOH} for inorganic gases have been determined by Bo *et al.*[8] and for a number of organic compounds by Park *et al.*;[9] most of the other values were calculated from reported activity coefficients, as shown in Table 2. For a number of solids, log L^{PrOH} and log L^{W} could be obtained from the solubility in propan-1-ol[10–16] and in water,[17–20] and the saturated vapour pressure of the solid at 298 K,[21] as the vapour concentration, C_G (Table 3). The relevant equations are

$$\log P^{PrOH/W} = \log L^{PrOH} - \log L^{W} = \log S_{PrOH} - \log S_{W} \qquad (5)$$

$$\log L^{PrOH} = \log S_{PrOH} - \log C_G \qquad (6)$$

$$\log L^{W} = \log S_{W} - \log C_G \qquad (7)$$

where S_{PrOH} and S_W are molar solubilities. Data for these solids are important, because the range of descriptor values is considerably increased. For all the solutes, a total of 79 log L^{PrOH} values could be obtained. The required descriptors in Eqn. (1) were available for all except fluoromethane, and 3-methylpyridine was a pronounced outlier. Descriptors for most of the solutes have been listed already,[1–6] and values for the remaining solutes are given in Table 4. Data for the 77 solutes led to the correlation equation

$$\begin{aligned}\log L^{PrOH} = {} & -0.028(0.025) - 0.185(0.062)R_2 + 0.648(0.087)\pi_2{}^{H} + 4.022(0.092)\Sigma\alpha_2{}^{H} \\ & + 1.043(0.084)\Sigma\beta_2{}^{H} + 0.869(0.010)\log L^{16} \qquad (8) \\ & n = 77,\ r^2 = 0.9976,\ \mathrm{SD} = 0.12,\ F = 6073\end{aligned}$$

where the sd values for the coefficients are given in parentheses. Eqn. (8) is statistically good and could be used to predict further log L^{PrOH} values for solutes with known descriptors. Since we have all the descriptors in Eqn. (8) available for ca 3000 solutes, this might be of considerable use.

Comparison of the descriptors in Eqn. (8) with those listed in Table 1 shows that there is little difference in solubility properties amongst the three alcohols studied to date. Propan-1-ol is slightly less dipolar/polarizable than methanol or ethanol, and since propan-1-ol is likely to be the most polarizable, this implies that propan-1-ol is less

Copyright © 1999 John Wiley & Sons, Ltd.

Table 2. Values of log L^{PrOH}, log L^{W} and log $P^{\mathrm{PrOH/W}}$ for solutes at 298 K

Solute	log L^{PrOH}	log L^{W}[a]	log $P^{\mathrm{PrOH/W}}$[b]
Helium	−1.56[c]	−2.02	0.46
Neon	−1.41[c]	−1.96	0.55
Argon	−0.61[c]	−1.47	0.86
Krypton	−0.16[c]	−1.21	1.05
Xenon	0.38[c]	−0.97	1.35
Hydrogen	−1.12[c]	−1.72	0.60
Oxygen	−0.66[c]	−1.51	0.85
Nitrogen	−0.88[c]	−1.80	0.92
Nitrous oxide	0.44[d]	−0.23	0.67
Carbon monoxide	−0.75[d]	−1.62	0.87
Carbon dioxide	0.35[e]	−0.08	0.43
Methane	−0.29[c]	−1.46	1.17
Ethane	0.45[d]	−1.34	1.79
Butane	1.45[f]	−1.52	2.97
Pentane	1.81[g]	−1.70	3.51
Hexane	2.28[g]	−1.82	4.10
2-Methylpentane	2.15[h]	−1.84	3.99
Heptane	2.74[g]	−1.96	4.70
2,4-Dimethylpentane	2.43[h]	−2.08	4.51
Octane	3.17[g]	−2.11	5.28
2,2,4-Trimethylpentane	2.69[i,,j]	−2.12	4.81
2,3,4-Trimethylpentane	2.95[h]	−1.88	4.83
Nonane	3.55[k]	−2.30	5.85
2,5-Dimethylheptane	3.40[h]	−2.191	5.59
Cyclopropane	1.15[m]	−0.55	1.70
Cyclopentane	2.12[i,n]	−0.88	3.00
Cyclohexane	2.55[i,o]	−0.90	3.45
Ethylcyclohexane	3.28[h]	−1.591	4.87
Cycloheptane	3.13[i,n]	−1.391	4.52
Ethene	0.38[p]	−0.94	1.32
Fluoromethane	−0.02[q]	0.16	−0.18
Tetrafluoromethane	−0.76[c]	−2.29	1.53
Tetrachloromethane	2.75[r]	−0.06	2.81
1-Chlorobutane	2.63[s]	0.12	2.51
2-Chloro-2-methylpropane	2.06[t]	−0.80[u]	2.86
2-Bromo-2-methylpropane	2.34[t]	−0.59[t]	2.93
Iodoethane	2.56[v]	0.54	2.02
$CFCl_2CFCl_2$	2.67[w]	−0.64	3.31
Tetrahydrofuran	2.90[x]	2.55	0.35
1,4-Dioxane	3.27[y]	3.71	−0.44
Butanone	3.07[z]	2.72	0.35
Pentane-2,4-dione	3.69[s]		
Dimethyl carbonate	2.73[aa]	2.731	0.00
Methyl propanoate	2.85[ab]	2.15	0.70
Methyl butanoate	3.28[ab]	2.08	1.20
Ammonia	1.76[d]	3.15	−1.39
Dimethylamine	2.19[d]	3.15	−0.96
Trimethylamine	2.56[ac]	2.35	0.21
Triethylamine	3.50[v]	2.36	1.14
Nitromethane	2.85[y]	2.95	−0.10
Methanol	3.15[ad,ae]	3.74	−0.59
Ethanol	3.51[z]	3.67	−0.16
Propan-1-ol	3.98[af]	3.56	0.42
Propan-2-ol	3.67[ag]	3.48	0.19
Butan-1-ol	4.47[ad,ae]	3.46	1.01
Pentan-1-ol	4.97[ad,ah]	3.35	1.62
Decan-1-ol	7.13[ai]	2.67	4.46
Sulfur hexafluoride	−0.13[c]	−2.23	2.10
Tetramethyltin	2.52[aj]	−1.53[aj]	4.05
Tetramethyltin	4.47[aj]	−1.62[aj]	6.09
Tetraethyllead	4.69[aj]	−1.49[aj]	6.18
Benzene	2.78[ak]	0.63	2.15
Toluene	3.31[z]	0.65	2.66
trans-Stilbene	7.31[al]	2.78	4.53
Naphthalene	5.19[am]	1.73[am]	3.46
Acenaphthene	6.25[am]	2.36[am]	3.89
Anthracene	7.36[am]	3.03[am]	4.33
Phenanthrene	7.30[am]	2.80[am]	4.50
Pyrene	8.40[am]	3.50[am]	4.90
Benzyl chloride	4.41[y]	1.38	3.03
Benzyl bromide	4.70[y]	1.90	2.80
Methyl 4-aminobenzoate	8.14[am]	6.56[am]	1.58
4-Nitrobenzyl chloride	6.26[ac]	3.77[l]	2.49
4-Aminobenzoic acid			1.04[am]
2-Hydroxybenzoic acid	7.59[am]	5.35[am]	2.24
4-Hydroxybenzoic acid	8.40[am]	6.78[am]	1.62
Methyl 4-hydroxybenzoate	8.93[am]	6.84[am]	2.09
Pyridine	3.99[y]	3.44	0.55
3-Methylpyridine	4.65[an,ao]	3.50	1.15
Thiophene	2.72[ap]	1.04	1.68

[a] Values from Refs 1 and 22, unless shown otherwise.
[b] From Eqn. (3).
[c] Ref. 8.
[d] From the Solubility Data Project.
[e] Ref. 23.
[f] Ref. 24.
[g] Ref. 25.
[h] Ref. 26.
[i] Ref. 27.
[j] Ref. 28.
[k] Ref. 29.
[l] Calculated value, using Eqn. (i) in Ref. 1.
[m] Ref. 30.
[n] Ref. 31.
[o] Ref. 32.
[p] Ref. 33.
[q] Ref. 34.
[r] Ref. 35.
[s] Ref. 36.
[t] Ref. 37.
[u] Revised value.
[v] Ref. 38.
[w] Ref. 39.
[x] Ref. 40.
[y] Ref. 41.
[z] Ref. 9.
[aa] Ref. 42.
[ab] Ref. 43.
[ac] Ref. 44.
[ad] Ref. 45.
[ae] Ref. 46.
[af] Activity coefficient taken as unity.
[ag] Ref. 47.
[ah] Ref. 48.
[ai] Ref. 49.
[aj] Ref. 50.
[ak] Ref. 51.
[al] Ref. 52.
[am] From Table 3.
[an] Ref. 53.
[ao] Ref. 54.
[ap] Ref. 55.

Copyright © 1999 John Wiley & Sons, Ltd.

Table 3. Calculation of log L^{PrOH}, log L^{W} and log $P^{PrOH/W}$ for some solid solutes at 298 K

Solute	Log S_{PrOH}	Log S_W	Log C_G	Log L^{PrOH}	Log L^W	Log $P^{PrOH/W}$
Naphthalene	−0.15[a]	−3.61[b]	−5.34[c]	5.19	1.73	3.46
Acenaphthene	−0.65[d]	−4.54[b]	−6.90[c]	6.25	2.36	3.89
Anthracene	−2.10[e]	−6.43[f]	−9.46[c]	7.36	3.03	4.33
Phenanthrene	−0.67[a]	−5.17[g]	−7.97[c]	7.30	2.80	4.50
Pyrene	−1.25[h]	−6.15[b]	−9.65[c]	8.40	3.50	4.90
Methyl 4-aminobenzoate	0.20[i]	−1.38[i]	7.94[j]	8.14	6.56	1.58
4-Aminobenzoic acid						1.04[k]
2-Hydroxybenzoic acid	0.32[l]	−1.91[m]	−7.27[j]	7.59	5.35	2.24
4-Hydroxybenzoic acid	0.15[n]	−1.48[n]	−8.25[j]	8.40	6.78	1.62
Methyl 4-hydroxybenzoate	0.26[n]	−1.83[n]	8.67[j]	8.93	6.84	2.09

[a] Ref. 10.
[b] Refs. 17–19.
[c] Ref. 21.
[d] Ref. 11.
[e] Ref. 12.
[f] Ref. 18.
[g] Ref. 20.
[h] Ref. 13.
[i] Ref. 14.
[j] Calculated from Eqn. (i), Ref. 1.
[k] Ref. 56.
[l] Ref. 15.
[m] Ref. 57.
[n] Ref. 16.

dipolar. The hydrogen bond basicity of propan-1-ol is slightly higher than expected, being even larger than that of water. The hydrogen bond acidity of the alcohols decreases steadily from methanol to propan-1-ol, with all three alcohols being very much less acidic than water. As might be expected, the lipophilicity/hydrophobicity of propan-1-ol, judged by the *l* coefficient, is higher than for the other alcohols, but considerably less than that for chloroform, for example. Overall, the coefficients in Eqn. (8) are comparable to those for methanol or ethanol. The very large hydrogen bond basicities shown by the alcohols, with *a* coefficients close to that for water, and the low hydrogen bond acidities of the alcohols are therefore not 'one-off' artifacts, but are consistent observations, within the formalism of Eqn. (1).

The values of log L^W required to calculate log $P^{PrOH/W}$ through Eqn. (3) are available, mostly from reported collections of data,[1,22] and are given in Table 2 together with log $P^{PrOH/W}$ values. Apart from the two compounds not used in Eqn. (8), pentane-2,4-dione had to be excluded, as we had no log L^W value, and so we were left with 76 values of the water–propan-1-ol partition coefficient. Application of Eqn. (4) led to the correlation equation

$$\begin{aligned}\log P^{PrOH/W} = {} & 0.148(0.036) + 0.436(0.063)R_2 - 1.098(0.091)\pi_2{}^{H} + 0.389(0.092)\Sigma\alpha_2{}^{H} \\ & - 3.893(0.095)\Sigma\beta_2{}^{H} + 4.036(0.043)Vx \qquad (9) \\ & n = 76,\ r^2 = 0.9952,\ SD = 0.13,\ F = 2892\end{aligned}$$

Table 4. Descriptors for some solutes

Solute	R_2	$\pi_2{}^H$	$\sum\alpha_2{}^H$	$\sum\beta_2{}^H$	Vx	Log L^{16}
Dimethyl carbonate	0.142	0.61	0.00	0.55	0.6644	2.447
Methyl 4-aminobenzoate	1.028	1.52	0.32	0.59	1.1724	6.085
2-Hydroxybenzoic acid	0.890	0.84	0.71	0.38	0.9904	4.721
4-Hydroxybenzoic acid	0.930	0.90	0.81	0.56	0.9904	4.867
Methyl 4-hydroxybenzoate	0.900	1.37	0.69	0.45	1.1313	5.665
4-Aminobenzoic acid	1.075	1.57	0.90	0.65	1.0315	—

Copyright © 1999 John Wiley & Sons, Ltd.

Table 5. Coefficients in Eqn. (4) for partition from water to dry and wet alcohols

Solvent	c	r	s	a	b	v	$[H_2O]$[a]
Methanol	0.329	0.299	−0.671	0.080	−3.389	3.512	
Ethanol	0.208	0.409	−0.959	0.186	−3.645	3.928	
Propan-1-ol	0.148	0.436	−1.098	0.389	−3.893	4.036	
Pentan-1-ol, wet	0.175	0.575	−0.787	0.020	−2.837	3.249	3.36
Hexan-1-ol, wet	0.143	0.718	−0.980	0.145	−3.214	3.403	3.32
Octan-1-ol, wet	0.088	0.562	−1.054	0.034	−3.460	3.814	2.36
Decan-1-ol, wet	0.008	0.485	−0.974	0.015	−3.798	3.945	1.65

[a] Molar concentration of water in the water-saturated alcohol, from Ref. 59.

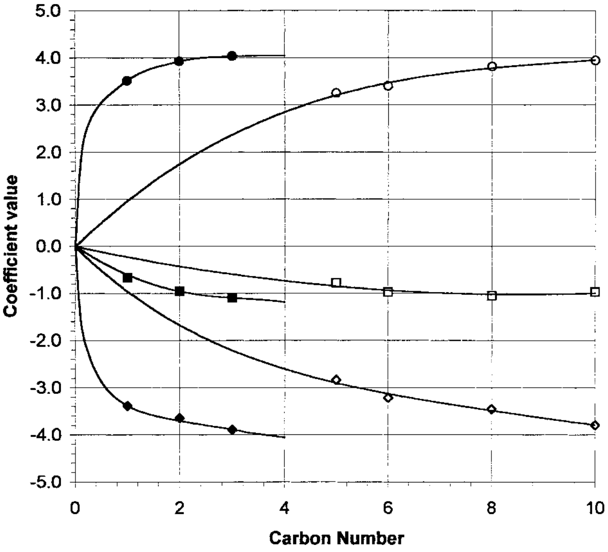

Figure 1. Plots of the coefficients in Eqn. (4) for partitions between water and dry alcohols ($n = 1$–3) and for partitions between water and wet alcohols ($n = 5$–10) against the carbon number of the alcohol: ●, ν-coefficient; ■, s-coefficient; ◆, b coefficient. Closed symbols are for the dry alcohols and open symbols for the wet alcohols

The statistics of Eqn. (9) are fairly good, in view of the fact that the error in the experimental log $P^{PrOH/W}$ value will include errors in both the log L^{PrOH} and log L^{W} values. The coefficients in Eqn. (9) now refer to the difference in properties of water and propan-1-ol. The positive r coefficient shows that dispersive interactions involving propan-1-ol are more important than those involving water. The negative s coefficient indicates that propan-1-ol is less dipolar/polarizable than is water; since propan-1-ol is more polarizable than water it is hence much less dipolar, at least as regards solubility interactions. The small a coefficient in Eqn. (9) confirms our deduction from Eqn. (8), namely that propan-1-ol is about as basic (in the hydrogen bond sense) as water, and the very negative b coefficient shows again that solvent propan-1-ol is a very much weaker hydrogen bond acid than is solvent water. Finally, the large v coefficient is in line with that observed for numerous water–solvent partitions,[58,59] and shows that propan-1-ol is somewhat hydrophobic.

We have previously compared[2,3] the hydrogen bond acidities and basicities of alcohols as obtained by the methods we use here with those obtained by the solvatochromic method of Kamlet, Taft and co-workers.[60,61] There is little to add to this comparison, save that the hydrogen bond propensities of propan-1-ol as deduced through Eqns (8) and (9) are in line with those of methanol and ethanol.

However, there are now enough data to compare coefficients in Eqn. (4) for partition between water and dry alcohols with those obtained for practical partitions between water and wet alcohols.[58,59] Coefficients in Eqn. (4) are given in Table 5 for water–solvent partitions, together with the molar solubility of water in the water-saturated alcohols.[59] There is no great change in the r and a coefficients on going from the dry to the wet alcohols, so that the presence of water in the wet alcohols has no effect on the hydrogen bond basicity of the solvent, possibly because water is itself of similar basicity to alcohols.[1–3] There are much larger effects on the other three coefficients, as shown in Fig. 1. Note that in Fig. 1, the zero coefficients for water at the point (0,0) are correct, because by definition they are all zero for transfer from water to water itself. However, the assignment of a carbon number of zero to water is arbitrary, and therefore so is the position of the point for water on the x-axis. This does not affect the general conclusions in any way. Addition of water to the alcohols makes the s coefficient slightly less negative, that is, the wet alcohols are slightly more dipolar than the dry alcohols. However, similar addition of water makes the b coefficient, that reflects the difference in hydrogen bond acidity of water and the alcohols, very much less negative, so that the wet alcohols are much stronger hydrogen bond acids than the dry alcohols. An almost mirror-image effect is shown by the change in the v coefficient; the wet alcohols have lower coefficients than expected from consideration of the dry alcohols, and so are less hydrophobic/lipophilic than expected. As the length of the alcohol chain increases, the solubility of water in the alcohol decreases, and the effect of water levels off. Indeed, from Fig. 1, we might predict that the solubility properties of dry decan-

Copyright © 1999 John Wiley & Sons, Ltd.

1-ol will be close to those of wet decan-1-ol. In particular, the hydrogen bond acidity of wet and dry decan-1-ol should be nearly the same, as should the hydrophobicity/lipophilicity.

In conclusion, we have shown that Eqns (1) and (4) can be applied to new sets of data on gas–propan-1-ol and water–propan-1-ol partitions. The correlation equations obtained are in accord with those we have found previously for methanol and ethanol, and can be used to deduce solubility-related properties of propan-1-ol, and to compare these properties with those of other dry and wet alcohols.

Acknowledgements

We are very grateful to Roche Products Limited for a research studentship (to J.L.).

REFERENCES

1. M. H. Abraham, J. Andonian-Haftvan, G. S. Whiting, A. Leo and R. W. Taft, *J. Chem. Soc., Perkin Trans. 2* 1777–1791 (1994).
2. M. H. Abraham, G. S. Whiting, P. W. Carr and H. Ouyang, *J. Chem. Soc., Perkin Trans. 2* 1385–1390 (1998).
3. M. H. Abraham, G. S. Whiting, W. J. Shuely and R. M. Doherty, *Can. J. Chem.* **76**, 703–709 (1998).
4. M. H. Abraham, *Chem. Soc. Rev.* **22**, 73–83 (1993).
5. M. H. Abraham, P. L. Grellier and R. A. McGill, *J. Chem. Soc., Perkin Trans. 2* 797–803 (1987).
6. M. H. Abraham, J. A. Platts, A. Hersey, A. J. Leo and R. W. Taft, *J. Pharm. Sci.*, submitted for publication.
7. M. H. Abraham and J. C. McGowan, *Chromatographia* **23**, 243–246 (1987).
8. S. Bo, R. Battino and E. Wilhelm, *J. Chem. Eng. Data* **38**, 611–616 (1993).
9. J. H. Park, A. Hussan, P. Couasnon, D. J. Fritz and P. W. Carr, *Anal. Chem.* **59**, 1970–1976 (1987).
10. A. Seidell, *Solubilities of Organic Compounds*, 3rd. ed. Van Nostrand, New York (1941); A Seidell and W. F. Linke, *Solubilities of Organic Compounds* 3rd. ed., Supplement, Van Nostrand, New York (1952).
11. C. L. Speyers, *Am. J. Sci.*, **14**, 293–302 (1902).
12. W. E. Acree Jr, *IUPAC Solubility Data Series*, Vol. 58. Oxford University Press, Oxford (1995).
13. M. E. R. Hale, K. S. Coym, K. A. Fletcher and W. E. Acree Jr, *J. Chem. Eng. Data*, **42**, 511–513 (1997).
14. P. Ruelle and U. W. Kesselring, *J. Pharm. Sci.* **87**, 987–997 (1998).
15. W. E. Acree, Jr, unpublished work.
16. A. Martin, P. L. Wu and A. Beerbower, *J. Pharm. Sci.* **73**, 188–194 (1984).
17. W. E. May, S. P. Wasik, M. M. Miller, Y. B. Tewari, J. B. Brown-Thomas and R. N. Goldberg, *J. Chem. Eng. Data* **28**, 197–200 (1981).
18. S. P. Wasik, M. M. Miller, Y. B. Tewari, W. E. May, W. J. Sonnefeld, H. DeVoe and W. H. Zoller, *Residue Rev.* **85**, 29–42 (1983).
19. R. S. Pearlman, S. H. Yalkowsky and S. Banerjee, *J. Phys. Chem. Ref. Data* **13**, 555–562 (1984).
20. D. Mackay and W. Y. Shiu, *J. Phys. Chem. Ref. Data* **10**, 1175–1199 (1981).
21. R. M. Stephenson and S. Malinowski, *Handbook of the Thermodynamics of Organic Compounds*. Elsevier, New York (1987).
22. S. Cabani, P. Gianni, V. Mollica and L. Lepori, *J. Solution Chem.* **10**, 563–595 (1981).
23. J. Tokunaga, *J. Chem. Eng. Data* **20**, 41–46 (1975).
24. Y. Mijyano and W. Hayduk, *J. Chem. Eng. Data* **31**, 77–80 (1986).
25. V. Dohnal and P. Vrba, *Fluid Phase Equilib* **133**, 73–87 (1997).
26. J. Gmehling, J. Menke and M. Schiller, *Activity Coefficients at Infinite Dilution Chemical Data Series*, Volume IX, Part 3. DECHEMA, Frankfurt/Main, (1978–84).
27. P. Vrbka, V. Dohnal, L. M. Trejo and M. Costas, *Fluid Phase Equilib* **137**, 133–140 (1997).
28. S. M. Ashraf, M. Ramakrishna and D. H. L. Prasad, *Phys. Chem. Liq.* **34**, 89–102 (1997).
29. H. Heitz, E. Dolch and R. N. Lichtenthaler, *Fluid Phase Equilib* **27**, 61–79 (1986).
30. C. E. Loeffler and J. J. McKetta Jr, *J. Chem. Eng. Data* **11**, 431–433 (1996).
31. T. M. Letcher, J. Mercer-Chalmers and A. K. Prasad, *Thermochim. Acta* **188**, 157–162 (1991).
32. I. Nagata and K. Kazuma, *J. Chem. Eng. Data* **22**, 79–84 (1977).
33. F. L. Boyer and L. J. Bircher, *J. Phys. Chem.* **64**, 1330–1331 (1960).
34. C. S. O. Silva, I. M. A. Fonseca and L. Q. Lobo, *Fluid Phase Equilib.* **135**, 137–144 (1997).
35. E. Matteoli and L. Lepori, *J. Chem. Thermodyn.* **18**, 1065–1076 (1986).
36. J. Gmehling, U. Onken and W. Arlt, *Vapor–Liquid Equilibrium Data Collection Chemical Data Series*, Volume I, Parts 2b–d. DECHEMA, Frankfurt/Main (1978–84).
37. M. H. Abraham, P. L. Grellier, A. Nasehzadah and R. A. C. Walker, *J. Chem. Soc., Perkin Trans. 2* 1717–1724 (1988).
38. M. H. Abraham and P. L. Grellier, *J. Chem. Soc., Perkin Trans. 2* 1735–1741 (1976).
39. V. Dohnal and M. Novotna, *Fluid Phase Equilib* **23**, 303–313 (1985).
40. J. A. Salas, E. L. Arancibia and M. Katz, *Can. J. Chem.* **75**, 207–211 (1997).
41. M. H. Abraham and P. L. Grellier, *J. Chem. Soc., Perkin Trans. 2* 1856–1863 (1975).
42. F. Comelli and R. Francesconi, *J. Chem. Eng. Data* **42**, 705–709 (1997).
43. J. Fernandez, C. Berro and M. I. P. Andrade, *Fluid Phase Equilib* **20**, 145–153 (1985).
44. M. H. Abraham, *J. Chem. Soc. B* 299–308 (1971).
45. P. Oracz, Int. DATA Ser., Sel. Data Mix. 75–77, 87–89, 96–98 (1986).
46. G. C. Benson, Int. DATA Ser., Sel. Data Mix. 77, 85 (1973).
47. J. Polak, S. Murakami, G. C. Benson and H. D. Pflug, *Can. J. Chem.* **48**, 3782–3785 (1970).
48. H. H. Sun, J. J. Christensen, R. M. Izatt and R. W. Hanks, *J. Chem. Thermodyn.* **12**, 95–99 (1980).
49. G. C. Benson, Int. DATA Ser., Sel. Data Mix. 92–94 (1985).
50. M. H. Abraham, *J. Chem. Soc., Perkin Trans. 2* 1343–1357 (1972).
51. I. Endler, G. Hradetzky and H.-J. Bittrich, *J. Prakt. Chem.* **327**, 693–697 (1985).
52. M. H. Abraham, C. Green, W. E. Acree Jr., C. E. Hernandez and L. E. Roy, *J. Chem. Soc., Perkin Trans. 2* 2677–2681 (1998).
53. S. Warycha, Int. DATA Ser., Sel. Data Mix. 130–132 (1994).
54. A. Orszagh and T. Kasprzycka-Guttman, *Bull. Acad. Pol. Sci., Ser. Chim.* **22**, 625–629 (1974).
55. J. O. Triday, *J. Chem. Eng. Data* **28**, 307–310 (1983).
56. H.-M. Lin and R. A. Nash, *J. Pharm. Sci.* **82**, 1018–1026 (1993).
57. A. Osol and M. Kilpatrick, *J. Am. Chem. Soc.*, **55**, 4440–4444 (1933).
58. M. H. Abraham, H. S. Chadha, G. S. Whiting and R. C. Mitchell, *J. Pharm. Sci.* **83**, 1085–1100 (1994).
59. M. H. Abraham, H. S. Chadha, J. P. Dixon and A. Leo, *J. Phys. Org. Chem.* **7**, 712–716 (1994).
60. M. J. Kamlet, J.-L. M. Abboud and R. W. Taft, *Prog. Phys. Org. Chem.* **13**, 485–630 (1981).
61. R. W. Taft, J.-L. M. Abboud, M. J. Kamlet and M. H. Abraham, *J. Solution Chem.* **14**, 153–186 (1985).

Copyright © 1999 John Wiley & Sons, Ltd.