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Physics and Chemistry of Liquids

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713646857>

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To cite this Article Prasad, T. E. Vittal, Sriram, N., Raju, A. N. and Prasad, D. H. L. (2005) 'Activity coefficients of the binary mixtures of *n*-decane with some aliphatic alcohols at 95.8 kPa', *Physics and Chemistry of Liquids*, 43: 4, 387 – 390

To link to this Article: DOI: 10.1080/00319100500132737

URL: <http://dx.doi.org/10.1080/00319100500132737>

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Activity coefficients of the binary mixtures of *n*-decane with some aliphatic alcohols at 95.8 kPa

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(Received 5 January 2005)

Activity coefficients at 95.8 kPa (over the whole composition range) are evaluated from the measurements on the bubble point temperatures of the binary mixtures of *n*-decane with: *iso*-propanol, *n*-butanol, *iso*-butanol, *sec*-butanol, *tert*-butanol and active amylalcohol. A Swietoslowski-type ebulliometer is used for the measurements. The Wilson model, found to represent the liquid phase composition *versus* temperature data well, is used for the calculations.

Keywords: Activity coefficients; Bubble point temperatures; Alcohols; *n*-Decane

1. Introduction

This investigation on the activity coefficients of the binary mixtures formed by decane with some aliphatic alcohols is in continuation of our studies leading to the phase equilibria of the binary mixtures containing hydrocarbons and alcohols [1,2]. The measurements on the bubble point temperatures needed for this purpose have been carried out at 95.8 kPa. We could not locate any experimental data in the literature on the systems chosen for the present study, for comparison purposes.

2. Experimental section

2.1. Method

A Swietoslowski-type ebulliometer, very similar to the one described by Hala *et al.* [3], is used for this experimental investigation. Connection of the ebulliometer to a good vacuum system, through a mercury manometer in-line, facilitated the creation and the maintenance of the chosen pressure to within ± 0.1 kPa. The equilibrium

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temperatures are measured to an accuracy of ± 0.1 K, by means of a platinum resistance thermometer, calibrated by means of point-to-point comparison with a Standard Platinum Resistance Thermometer certified by the National Bureau of Standards, Boulder (USA). Samples of liquid mixtures for the studies are prepared gravimetrically, making use of an electronic balance precise to ± 0.0001 g and stirring well before being placed in the ebulliometer. The heating rate is adjusted to yield the desired condensate drop rate of 30 drops per minute in accordance with the suggestion of Hala *et al.* [3]. Equilibrium temperatures, measured after the steady drop rate and constant temperature are maintained for at least 30 min, are reported.

2.2. Materials

AR-grade chemicals used in this study are further purified according to the easiest possible of the methods described in Riddick *et al.* [4]. The purity of the chemicals is ascertained by measuring their density and refractive index, which compare well with the literature values [4] as shown in table 1.

3. Results and discussion

The experimental liquid phase composition (x_1) versus temperature (T) data, summarized in table 2, are fitted to the Wilson [5] model. The optimum Wilson parameters are obtained by minimizing the objective function defined as

$$\varphi = \sum \left[\frac{P_{\text{cal}}}{P_{\text{expt}}} - 1 \right]^2 \quad (1)$$

where P_{cal} and P_{expt} stand for the calculated and experimental total pressures. The Nelder–Mead optimization technique described by Kuester and Mize [6] is used. Vapor pressures needed in the computations are calculated from the Antoine constants in table 3. The Antoine equation, with the constants noted in table 3, represents the literature vapor pressure data as well as the present measurements on pure liquids with an average absolute deviation of 0.5%. The molar volumes of the pure liquids, calculated from the density values of this study (table 1) are used as the input in

Table 1. Comparison of the density (d) and refractive index (n) of the pure substances with literature data [4] at 298.15 K.

Substance	d (kg m ⁻³)		n_D	
	This work	Literature	This work	Literature
<i>n</i> -Decane	726.4	726.35	1.4097	1.40967
<i>iso</i> -Propanol	781.3	781.26	1.3752	1.37520
<i>n</i> -Butanol	805.8	805.75	1.3974	1.39741
<i>iso</i> -Butanol	797.8	797.80	1.3939	1.39389
<i>sec</i> -Butanol	802.4	802.41	1.3953	1.39530
<i>tert</i> -Butanol	781.2	781.20	1.3852	1.38520
Active amylalcohol	810.8	810.80	1.4080	1.40800

Table 2. Bubble point temperatures and activity coefficients at 95.8 kPa.

x_1	T (K)	γ_1	γ_2	x_1	T (K)	γ_1	γ_2	x_1	T (K)	γ_1	γ_2
<i>iso</i> -Propanol(1) + <i>n</i> -decane(2)				<i>n</i> -Butanol(1) + <i>n</i> -decane(2)				<i>iso</i> -Butanol(1) + <i>n</i> -decane(2)			
0.0000	445.25	3.3104	1.0000	0.0000	445.25	1.3880	1.0000	0.0000	445.25	2.3153	1.0000
0.1752	378.85	2.6715	1.0363	0.1369	424.15	1.2160	1.0098	0.1752	402.35	2.0050	1.0190
0.2981	363.85	2.1633	1.1116	0.3225	411.25	1.0918	1.0419	0.2981	392.95	1.7749	1.0618
0.4593	359.55	1.6870	1.3002	0.5085	403.15	1.0346	1.0812	0.4593	386.75	1.5111	1.1769
0.8360	355.75	1.0904	3.1502	0.6513	398.45	1.0137	1.1110	0.8360	381.05	1.0788	2.3862
0.9386	354.85	1.0168	5.5949	0.7920	394.45	1.0039	1.1381	0.9386	380.15	1.0148	3.9454
1.0000	354.05	1.0000	9.8586	0.9195	391.25	1.0005	1.1600	1.0000	379.75	1.0000	6.5090
				1.0000	389.45	1.0000	1.1723				
<i>sec</i> -Butanol(1) + <i>n</i> -decane(2)				<i>tert</i> -Butanol(1) + <i>n</i> -decane(2)				Active amylalcohol(1) + <i>n</i> -decane(2)			
0.0000	445.25	3.6906	1.0000	0.0000	445.25	2.3978	1.0000	0.0000	445.25	11.5579	1.0000
0.1502	391.55	2.7140	1.0374	0.1373	384.85	2.1171	1.0181	0.1311	414.15	2.9459	1.0862
0.3466	381.35	1.7962	1.1963	0.3870	366.85	1.5156	1.1601	0.3116	409.95	1.5785	1.2837
0.4692	378.75	1.4793	1.3712	0.5601	362.25	1.2593	1.3787	0.4751	407.15	1.2334	1.5020
0.7609	374.75	1.0923	2.2504	0.7563	358.65	1.0825	1.8616	0.5469	406.05	1.1545	1.6096
0.9271	372.45	1.0093	3.4964	0.8324	357.35	1.0404	2.1766	0.7636	402.95	1.0321	1.9817
1.0000	371.35	1.0000	4.4980	0.9254	355.75	1.0085	2.7450	0.9157	401.15	1.0036	2.2902
				1.0000	354.25	1.0000	3.4479	1.0000	400.35	1.0000	2.4800

Table 3. Antoine constants for the equation $\ln(P/\text{kPa}) = A - B/[(T/\text{K}) + C]$.

Substance	<i>A</i>	<i>B</i>	<i>C</i>
<i>n</i> -Decane	13.9941	3456.78	-78.67
iso-Propanol	16.6755	3640.20	-53.54
<i>n</i> -Butanol	15.1985	3137.01	-94.53
iso-Butanol	14.8538	2874.72	-100.30
sec-Butanol	15.1928	3026.03	-86.65
tert-Butanol	14.8374	2658.51	-95.45
Amylalcohol	14.2435	2752.18	-116.30

Table 4. Representation of the measurements by the Wilson model.

System	$[(\lambda_{12} - \lambda_{11})/R]/\text{K}$	$[(\lambda_{12} - \lambda_{22})/R]/\text{K}$	Std. Dev. in <i>T</i> /K
iso-Propanol(1) + <i>n</i> -decane(2)	233.92	622.00	0.05
<i>n</i> -Butanol(1) + <i>n</i> -decane(2)	388.43	-209.08	0.04
iso-Butanol(1) + <i>n</i> -decane(2)	703.71	642.05	0.04
sec-Butanol(1) + <i>n</i> -decane(2)	391.30	291.61	0.02
tert-Butanol(1) + <i>n</i> -decane(2)	213.50	262.22	0.04
Amylalcohol(1) + <i>n</i> -decane(2)	1143.13	-535.04	0.03

obtaining the optimum Wilson parameters. The results of the representation of the phase equilibrium data by the Wilson [5] model, summarized in table 4, indicate that the data and the representation are quite good. The activity coefficients evaluated from the model are also given in table 2.

The results indicate that the activity coefficients of the more volatile components are generally in the order: active amylalcohol > sec-butanol > iso-propanol > tert-butanol > iso-iso-butanol > n-butanol, though no specific reason could be attributed to the behaviour. The data and the representation presented in the article are expected to be useful for engineering design purposes.

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