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Application of the ERAS model to volumetric properties of binary mixtures of banana oil with primary and secondary alcohols (C1–C4) at different temperatures

Mahboobe Behroozi, Hosseinali Zarei *

Faculty of Chemistry, Bu-Ali Sina University, Hamedan, Iran

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ABSTRACT

The densities of binary mixtures of {isoamyl acetate + alcohols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, and 2-butanol)}, including those of pure liquids, over the entire composition range were measured at temperatures (293.15 to 333.15) K and atmospheric pressure by means of a vibrating-tube densimeter. The excess molar volume, V_m^E, thermal expansion coefficients, α, and their excess values, α^E, were calculated from density data. The V_m^E values are positive over the entire range of composition and temperature and become more positive with increasing temperature for all of the mixtures except for the (isoamyl acetate + methanol) mixture. The V_m^E values were correlated by Redlich–Kister equation and the extended real associated solution (ERAS) model was used for describing V_m^E values at $T = 303.15$ K.

1. Introduction

Recently, investigation of the thermophysical properties of esters, due to their widespread use in industrial processes has increased. Esters are used in flavouring, perfuming, artificial essences, cosmetics, and also they are important solvents in pharmaceutical, paint, and plastic industries [1]. Isoamyl acetate known as banana oil is used as solvent for old colours, perfuming, shoe polish, metallic paints, and photographic films [2].

Despite the increasing investigation on esters, few studies have been reported on thermodynamic properties (density, V_m^E, thermal expansion, and so on) of isoamyl acetate binary mixtures as well as modelling with theoretical models. A literature survey shows that no data for ERAS model of the binary mixtures containing isoamyl acetate have been reported. Therefore, we are interested in the examination of the ERAS model for these mixtures. The ERAS model [3–5] combines the associated solution model [6,7] with Flory's equation of state [8]. The combined model has two terms: a physical term, related to the van der Waals interactions and a chemical term, related to association effect for self-associated solvents and cross-associated between unlike molecules in mixtures.

In this work, we report densities, V_m^E, thermal expansion coefficients α, and their excess values α^E, for binary mixtures of {isoamyl acetate + alcohols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, and 2-butanol)}, over the entire composition range at temperatures (293.15 to 333.15) K and atmospheric pressure. The V_m^E values were correlated by Redlich–Kister equation and the extended real associated solution (ERAS) model was used for describing V_m^E values at $T = 303.15$ K.

2. Experimental

2.1. Materials

The mass fraction purity and source of the materials are as follows. Isoamyl acetate ($\geqslant$0.99, Merck), methanol (0.998, Merck), ethanol (0.999, Merck), 1-propanol (0.998, Merck), 2-propanol (0.995, BDH), 1-butanol (0.998, Merck), and 2-butanol (0.99, Aldrich) were used without further purification. The purities declared by the manufacturer were ascertained by comparing their densities and refractive indices with the literature values [1,9–18]. Table 1 contains the experimental and literature values of the densities and refractive indices for the pure compounds at different temperatures.

2.2. Apparatus and procedure

Density measurements for pure components and binary mixtures were carried out with an Anton Paar digital vibrating u-tube densimeter (model DMA 4500) with an uncertainty of $5 \cdot 10^{-5}$ g · cm^{-3}. The temperature in the cell was regulated to ±0.01 K with a solid state thermostat (Peltier). The measurements were performed at temper-

* Corresponding author. Tel./fax: +98 0811 8257407.
E-mail address: zareih@basu.ac.ir (H. Zarei).

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TABLE 1
Comparison of densities ρ, refractive indices n_D^{25}, and thermal expansion coefficients α, of the pure components with literature values at different temperatures.

Component	T/K	$\rho/(g \cdot cm^{-3})$		n_D^{25}		$\alpha/(kK^{-1})$
		Experimental	Literature	Experimental	Literature	
Isoamyl acetate	293.15	0.87291	0.87295[a]	1.3975	1.3981[k]	1.118
	298.15	0.86800	0.86791[a]			1.127
	303.15	0.86313	0.86298[a]			1.136
	313.15	0.85329	0.85300[a]			1.158
	323.15	0.84337	0.84303[a]			1.181
	333.15	0.83337	0.83305[a]			1.204
Methanol	293.15	0.79138	0.79140[b]	1.3257	1.32652[k]	1.189
	303.15	0.78195	0.78190[c]			1.210
	313.15	0.77243	0.77250[c]			1.241
	323.15	0.76277	0.76286[c]			1.277
	333.15	0.75294				1.318
Ethanol	293.15	0.78950	0.78940[b]	1.3583	1.35941[k]	1.086
	303.15	0.78089	0.78073[d]			1.109
	313.15	0.77216	0.77198[d]			1.141
	323.15	0.76325	0.76210[e]			1.182
	333.15	0.75410				1.232
1-Propanol		0.80361	0.80363[f]	1.3822	1.3837[k]	0.990
	303.15	0.79558	0.79555[g]			1.019
	313.15	0.78740	0.78730[h]			1.049
	323.15	0.77904	0.77930[c]			1.088
	333.15	0.77042	0.77042[i]			1.141
2-Propanol		0.78516	0.78507[g]	1.3741	1.3752[k]	1.060
	303.15	0.77669	0.77660[g]			1.110
	313.15	0.76790	0.76780[h]			1.168
	323.15	0.75873	0.75868[i]			1.237
	333.15	0.74910	0.74906[i]			1.320
1-Butanol	293.15	0.80989	0.80980[b]	1.3964	1.3973[k]	0.937
	303.15	0.80224	0.80221[j]			0.962
	313.15	0.79445	0.79442[j]			0.990
	323.15	0.78649	0.78645[j]			1.025
	333.15	0.77831	0.77828[j]			1.068
2-Butanol	293.15	0.80676	0.80684[g]	1.3943	1.395[k]	1.015
	303.15	0.79843	0.79835[j]			1.063
	313.15	0.78975	0.78965[j]			1.125
	323.15	0.78065	0.78055[j]			1.194
	333.15	0.77110	0.77099[j]			1.268

[a] Interpolated from [1].
[b] Reference [9].
[c] Reference [10].
[d] Reference [11].
[e] Reference [12].
[f] Reference [13].
[g] Reference [14].
[h] Reference [15].
[i] Reference [16].
[j] Reference [17].
[k] Reference [18].

atures (293.15 to 333.15) K. The refractive indices were measured at T = 298.15 K with an Abbé refractometer with an uncertainty of ±0.0002 and for the temperature of measurement it was ±0.01 K. Before the measurements were taken, the apparatus was checked by double distilled water and dry air. All pure components were degassed with an ultrasonic cleaner just before the measurements. The mixtures were prepared in dark airtight stopper bottles by mass, using a Mettler AB 204-N balance accurate to ±0.1 mg, in an entire range of composition. The details of the used methods in our laboratory are given elsewhere [16]. The uncertainty of the mole fraction was less than $\pm 1 \cdot 10^{-4}$.

3. Results and discussions

3.1. Experimental

The measured densities of six binary mixtures containing {isoamyl acetate + (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, and 2-butanol)} at different temperatures were used to calculate V_m^E. The V_m^E values were calculated by equation (1) and the results are reported in table 2

$$V_m^E = \sum_{i=1}^{2} x_i M_i (\rho^{-1} - \rho_i^{-1}), \quad (1)$$

where x_i, M_i, ρ_i, and ρ are mole fraction of component i, molecular mass of the pure component, density of the pure component, and density of the mixture, respectively. The uncertainty in the determination of V_m^E was $\pm 2 \cdot 10^{-3}$ cm$^3 \cdot$ mol^{-1}. Redlich–Kister equation [19] was employed to correlate the results according to equation (2). Experimental data and the results obtained from Redlich–Kister equation as a function of the mole fraction of component 1 (isoamyl acetate) are represented in figures 1 to 3

$$V_m^E = x_1(1 - x_1) \sum_{i=0}^{k} A_i (1 - 2x_1)^i, \quad (2)$$

where x_1 is the mole fraction of component 1 (isoamyl acetate) and the adjustable parameters, A_i, were derived by least squares method.

There is a relation for temperature dependence of these fitting parameters [16]:

$$A_i = \sum_{j=0}^{2} B_{ij} T^j. \quad (3)$$

The parameters, B_{ij}, are temperature independent. The values of B_{ij} are given in table 3, along with standard deviation, σ, obtained by the method of least squares using the following equation: