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Densities and volumetric properties of 1,4-dioxane with ethanol, 3-methyl-1-butanol, 3-amino-1-propanol and 2-propanol binary mixtures at various temperatures

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ABSTRACT

Densities (ρ), viscosities (η), and refractive indexes (n_D) have been measured over the whole composition range for the binary mixtures of 1,4-dioxane with ethanol, 3-methyl-1-butanol, 3-amino-1-propanol and 2-propanol at 298.15, 303.15 and 308.15 K along with the properties of the pure components. By using the experimental values of ρ, η, and n_D, excess molar volume (V_m^E), partial molar volume ($\bar{v}_i$) and excess partial molar volumes ($\bar{v}_i^E$) of the binary mixtures have been calculated. The numerical values of V_m^E were fitted to the Redlich–Kister polynomial equation and other volumetric properties were calculated. The McAllister equation has also been used to correlate the viscosity data. The variations of these parameters with composition were discussed from the point of view of intermolecular interactions in the binary mixtures.

1. Introduction

Liquid mixtures frequently appear in chemical research. Most of the mixtures are non-ideal and show peculiar behavior. The interpretation of non-ideality is a fascinating area and a large number of contributions were made over the last decade on this topic. Solution theory is still far from enough to account for solution nonidealities in terms of the constituent molecules properties [1]. The volumetric properties of mixed solvent systems and their dependence on composition find different applications in many important chemical, industrial, and biological processes. The study of functions such as excess molar volume, partial molar volume and excess partial molar volumes of binary liquid mixtures is useful in understanding the nature and strength of molecular interactions between the component molecules. 1,4-Dioxane is a cyclic ether that has electron-donor ability due to two ion pairs of electrons on each oxygen atom. 1,4-Dioxane is an excellent aprotic solvent having a zero dipole moment and is commercially used in polymerization and other chemical reactions in the cleaning of polymer surfaces and electronic materials [2–4].

Alcohols are organic liquids and are widely used as the basic organic compound for the syntheses of other chemicals. The study of binary mixtures containing alcohol as one of the components has paid great attention due to a number of factors like (i) self-association of alcohol and (ii) change in the extent and strength of H-bonding in the mixture, which affect the values of their thermodynamic properties [5]. Mixtures containing alkanol amines are well-known for their ability to remove acidic components such as CO_2 and H_2S from gas stream. The amines are commonly used in oil refineries, in petroleum chemical plants, and in ammonia factories [6]. A knowledge of the various thermodynamic properties of mixtures involving cyclic ethers with self-associated alcohols and/or amino alcohols helps in designing an efficient industrial process and also in understanding variable types of molecular interactions. Several works [7,8] have been conducted about examining thermo-physical properties of binary liquid mixtures containing cyclic ethers. The second component was either an inert compound or a highly self-associated alcohol. In this study, we have reported density and viscosity measurements of the binary compositions including 1,4-dioxane at 298.15, 303.15 and 308.15 K. The dependence of ρ, η, and n on the composition of the mixtures has been checked by using an empirical relation. The experimental values of ρ were used to calculate some important thermodynamic quantities.

2. Experimental

2.1. Materials

The mole fraction purity of the components from Fluka was: 1,4-dioxane (≥98%), ethanol (96%), 3-methyl-1-butanol (≥99%) and 2-propanol (99.7%). All reagents were used without further purification. Binary mixtures were prepared by known masses of each liquid in air-

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Table 1
Properties characterizing the pure components at 298.15 K.

Component	ρ (g cm^{-3})		η (mPa s)		n_D	
	Exp	Lit	Exp	Lit	Exp	Lit
1,4-Dioxane	1.0279	1.02797 [9]	1.187	1.181 [10]	1.4200	1.4200 [11]
2-Propanol	0.7820	0.7812 [12]	2.189	2.081 [13]	1.3750	1.3752 [14]
3-Amino-1-Propanol	0.9873	0.98 [15][a]				
3-Methyl-1-butanol	0.8050	0.80439 [9]	3.7240	3.738 [9]	1.4050	1.4052 [16]

[a] At 293.15 K.

tight stopper glass bottles. In order to verify the calibration, the properties characterizing the pure components were compared with the literature values [9–16] in Table 1.

2.2. Instruments

Samples were prepared by mass using a single pan Precisa (240A) balance to an accuracy of ±0.0001 g. No buoyancy corrections were applied. The possible error in mole fraction is calculated to be less than $\pm 1\times10^{-4}$. Densities of the pure liquids and mixtures were measured using a digital vibrating glass tube densimeter (DA-500E, Japan). It was calibrated with double-distilled water and air. Kinematic viscosities were determined using a viscometer well equipped with a Schott–Gerate automatic measuring unit model AVS 400 having a transparent thermostat which allows temperature stabilization with a tolerance of 0.01 K. Capillary diameters of 0.63 and 0.84 mm were used for kinematic viscosity ranges of 1.2–10 and 3–30 cSt. Each time 15 cm^3 of solution was measured. The calibration was carried out with double distilled water and glycerol (60% w/v). The uncertainty of the viscosity measurement was ±0.7%. The refractive indices of pure liquids and their binary mixture were measured by using a thermostated Abbe refractometer. The values of refractive index were obtained for sodium D light.

3. Results and discussion

The densities (ρ),viscosities (η), refractive indices (n_D), excess molar volume (V^E_m), partial molar volume ($\bar{v}_i$) and excess partial molar volumes ($\bar{v}^E_i$) for the binary mixtures of 1,4-dioxane with

Table 2
Mole fractions (x_1), densities (ρ),viscosities (η), refractive indices (n_D), excess molar volumes (V^E_m), partial molar volume($\bar{v}_i$) and excess partial molar volumes ($\bar{v}^E_i$) of 1,4-dioxane + 2-propanol at 298.15, 303.15 and 308.15 K.

X_1	ρ (g cm^{-3})	η (mPa s)	n_D	V^E_m (cm^3 mol^{-1})	$\bar{v}_1$ (cm^3 mol^{-1})	$\bar{v}_2$ (cm^3 mol^{-1})	$\bar{v}^E_1$ (cm^3 mol^{-1})	$\bar{v}^E_2$ (cm^3 mol^{-1})
298.15 K								
0	1.0279	1.1876	1.4200	0	80.17694	85.71846	3.32272	0
0.1382	0.9936	1.0709	1.4142	0.29111	78.11072	85.85476	1.25650	0.13630
0.2768	0.9611	1.0345	1.4086	0.34021	76.9248	86.16187	0.07058	0.44341
0.3911	0.9354	1.0096	1.4042	0.23223	76.21281	86.51183	−0.69141	0.79337
0.4934	0.9126	1.0020	1.4001	0.06301	75.86018	86.81098	−0.99404	1.09252
0.5928	0.8907	1.0137	1.3958	−0.18411	75.78250	86.82652	−1.07172	1.10806
0.6977	0.8661	1.0808	1.3909	−0.36322	76.05033	86.37230	−0.80389	0.65384
0.7841	0.8443	1.2165	1.3867	−0.42301	76.39235	85.43658	−0.46187	−0.28188
0.8535	0.8259	1.4158	1.3831	−0.41923	76.61138	84.27162	−0.24284	−1.44684
0.9290	0.8039	1.7227	1.3789	−0.25101	76.80573	82.81758	−0.04849	−2.90088
1	0.7820	2.1899	1.3750	0	76.85422	81.51516	0	−4.20330
303.15 K								
0	1.0223	1.0938	1.4182	0	82.02101	86.18801	4.69214	0
0.1382	0.9871	0.9888	1.4124	0.37801	78.72268	86.40312	1.39381	0.21511
0.2768	0.9550	0.9414	1.4065	0.40300	77.19481	86.79657	−0.13406	0.60856
0.3911	0.9300	0.9353	1.4016	0.23963	76.54269	87.08652	−0.78618	0.89851
0.4934	0.9072	0.9403	1.3972	0.07502	76.36164	87.27812	−0.96723	1.09011
0.5928	0.8852	0.9543	1.3928	−0.16011	76.39845	87.14931	−0.93042	0.96130
0.6977	0.8602	1.0140	1.3880	−0.29849	76.70588	86.63846	−0.62299	0.45045
0.7841	0.8383	1.1121	1.3839	−0.34001	76.99954	85.80922	−0.32933	−0.37879
0.8535	0.8199	1.2589	1.3806	−0.32212	77.17050	84.91187	−0.15837	−1.27614
0.9290	0.7983	1.4697	1.3768	−0.18200	77.30427	83.94656	−0.02460	−2.24145
1	0.7772	1.7880	1.3732	0	77.32887	83.32189	0	−2.86612
308.15 K								
0	1.0166	1.0140	1.4155	0	83.19722	86.67126	5.47835	0
0.1382	0.9808	0.9165	1.4098	0.45215	79.38469	86.92878	1.66582	0.25752
0.2768	0.9490	0.8803	1.4040	0.47701	77.47183	87.42539	−0.24704	0.75413
0.3911	0.9250	0.8656	1.3990	0.26836	76.79635	87.70453	−0.92252	1.03327
0.4934	0.9023	0.8625	1.3944	0.08301	76.74085	87.78765	−0.97802	1.11639
0.5928	0.8801	0.8778	1.3900	−0.12021	76.92745	87.52820	−0.79142	0.85694
0.6977	0.8551	0.9221	1.3853	−0.23744	77.27187	86.91748	−0.44700	0.24622
0.7841	0.8330	1.0123	1.3815	−0.24602	77.53410	86.20279	−0.18477	−0.46847
0.8535	0.8147	1.1284	1.3784	−0.22914	77.63942	85.57003	−0.07945	−1.10123
0.9290	0.7935	1.3078	1.3750	−0.11101	77.71834	85.11466	−0.00053	−1.55660
1	0.7733	1.5704	1.3718	0	77.71887	85.12981	0	−1.54145