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Density and speed of sound for binary mixtures of 1,4-dioxane with propanol and butanol isomers at different temperatures

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ABSTRACT

The densities, ρ and the speeds of sound, u, for binary liquid mixtures of 1,4-dioxane with 1-propanol, 2-propanol, 1-butanol, and 2-butanol have been measured as a function of composition using an Anton-Paar DSA 5000 densimeter at temperatures (293.15, 298.15, 303.15 and 308.15) K and atmospheric pressure. The excess molar volumes, V^E, and excess molar isentropic compressibilities, $K^E_{S,m}$, were calculated from the experimental data. The computed quantities were fitted to Redlich–Kister equation to derive the coefficients and estimate the standard error values. Also, apparent molar volume, $V_{\phi,i}$ and partial molar volume, $\overline{V}_i$, excess partial molar volume, $\overline{V}^E_i$ and their limiting values at infinite dilution, $\overline{V}^0_{\phi,i}$, $\overline{V}^0_i$ and $\overline{V}^{E,\infty}_{m,i}$ respectively have been calculated from the experimental density measurements. Excess partial molar isentropic compression, $K^E_{S,i}$, of both components and their respective limits at infinite dilution, $K^{E,\infty}_{S,i}$, were analytically obtained using Redlich–Kister type equations. The variation of these properties with composition and temperature of the mixtures are discussed in terms of molecular interactions.

1. Introduction

1,4-Dioxane is a cyclic molecule used in variety of applications in industrial sectors e.g. as a stabilizer for storing and transporting 1,1,1-trichloroethane in aluminium containers, and in a variety of applications as a solvent, e.g. in inks and adhesives. Also, oxygenated compounds such as ethers and alcohols are used as gasoline additives and have been extensively investigated due to their great industrial interest [1]. Interactions of 1,4-dioxane with different types of liquids as studied by various researchers in previous years [2–12] are important from a fundamental viewpoint. Although the excess properties of 1,4-dioxane with n-alkanols have been measured by some researchers mainly at 298.15 K [13–20], references for the acoustic properties of 1,4-dioxane with n-alkanols at different temperature are scare.

As a part of our ongoing programme of research on thermodynamic and acoustic properties of binary liquid mixtures containing linear cyclic ethers, we report here the experimental data for density and speed of sound of binary mixtures of cyclic ether with 1-propanol, 2-propanol, 1-butanol, and 2-butanol and those of pure liquids at temperatures (293.15, 298.15, 303.15 and 308.15) K and atmospheric pressure over the entire composition range. The results will enable us to comprehend the effect of specific interactions on the excess properties, the dependence on the position of the OH group and the alkyl chain length in the alcohol, and also the influence of temperature on the composition dependent behaviour of these mixtures. An attempt is also made to ascertain whether the thermophysical properties of the cyclic ether + alkanol resemble those of linear ether + alkanol [21,22].

2. Experimental

2.1. Materials

1-Propanol, 2-propanol, 1-butanol, and 2-butanol (all S D Fine Chemicals, India, spectroscopic and analytical grade) were stored over sodium hydroxide pellets for several days and fractionally distilled twice [19]. The middle fraction of the distillate was used. 1,4-Dioxane (Acros, USA) was used without further purifications. Prior to experimental measurements, all liquids were stored in dark bottles over 0.4 nm molecular sieves to reduce water content, and were partially degassed with a vacuum pump under a nitrogen atmosphere. The estimated purities determined by gas chromatographic analysis were better than 99.5 mol% for all the liquid samples. The water content, measured by Karl-Fischer titration for each sample, was always found to be less than 0.002 mass %. The details of the chemicals used in the present work are also given in Table 1. Further, the purities of liquids were checked by comparing their densities and speeds of sound with their corresponding literature values [5,8,13,16,20,24–34] and are reported in Table 2. The experimental and literature values compare well in general.

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Table 1
Specification of chemical samples.

Chemical name	Provenance	CAS number	Purity (supplier)	Purity (GC)	Water content (supplier)	Water content (KF)
1,4-Dioxane	Acros, USA	123-91-1	≥0.995	>0.995	≤0.1%	<0.002%
1-Propanol	SD Fine Chem Ltd, India	71-23-8	>0.995	>0.995	0.1%	<0.002%
2-Propanol	SD Fine Chem Ltd, India	67-63-0	>0.995	>0.995	0.1%	<0.002%
1-Butanol	SD Fine Chem Ltd, India	71-36-3	>0.995	>0.995	0.1%	<0.002%
2-Butanol	SD Fine Chem Ltd, India	78-92-2	>0.995	>0.995	0.1%	<0.002%

2.2. Apparatus and procedure

The densities, ρ and speeds of sound, u, of both pure liquids and of the mixtures were simultaneously, and automatically measured, using an Anton Paar DSA 5000 densimeter. Both the density and speed of sound are extremely sensitive to temperature, so it was controlled to $\pm 1 \times 10^{-2}$ K by built-in solid state thermostat. Before each series of measurements, the apparatus was calibrated with double-distilled and degassed water, n-hexane, n-heptane, n-octane, cyclohexane, and benzene. The sensitivity of the instrument corresponds to a precision in density and speed of sound measurements of 1×10^{-6} g cm^{-3} and 1×10^{-2} m s^{-1}. The uncertainty of the density and speed of sound are $\pm 3 \times 10^{-6}$ g cm^{-3} and $\pm 1 \times 10^{-1}$ m s^{-1}, respectively.

The mixtures were prepared by mass and were kept in special airtight stoppered glass bottles to avoid evaporation. The weighings were done on an A&D company limited electronic balance (Japan, Model GR-202) having a precision of ± 0.01 mg. The probable error in the mole fraction was estimated to be less than $\pm 1 \times 10^{-4}$. All molar quantities were based on the IUPAC relative atomic mass table [35].

3. Equations

3.1. Ultrasonic speeds and isentropic compressibilities

With the assumption that the absorption of the acoustic wave is negligible [36], the isentropic compressibility, κ_S, can be calculated using the Newton–Laplace's equation:

$$\kappa_S = 1/u^2\rho = V\left(Mu^2\right)^{-1}. \tag{1}$$

The molar isentropic compressibilities $K_{S,m}$, can be obtained from Eq. (2):

$$K_{S,m} = -(\delta V/\delta P)_s = V\kappa_S = \Sigma x_i M_i/(\rho u)^2, \tag{2}$$

where ρ is the density, V, is the molar volume, and x_i and M_i are the mole fraction and molar mass of component i in the mixture, respectively.

Table 2
Thermodynamic parameter for pure components.

Component	T/(K)	$\rho \times 10^3/(\text{kg·m}^{-3})$ Exp.	Lit.	$\alpha \times 10^{-3}/(\text{K}^{-1})$	$C_P^*/(\text{J·mol}^{-1}\text{·K}^{-1})$	$u/(\text{m·s}^{-1})$ Exp.	Lit.	$K_{S,m}^* \times 10^9/(\text{m}^3\text{·mol}^{-1}\text{·MPa}^{-1})$
1,4-Dioxane	293.15	1.033782		1.096[a]	148.68[b]	1367.26		44.101
	298.15	1.028118	1.02809 [5] 1.0283 [8] 1.02797 [16]	1.102[a]	150.61 [18]	1344.20	1345 [8] 1345.5 [16]	46.131
	303.15	1.022455	1.0283 [8] 1.02230 [13] 1.0223 [20]	1.119[a]	152.56[b]	1321.83		48.236
	308.15	1.01668	1.0178 [8]	1.136[a]	154.59[b]	1300.34		50.411
1-Propanol	293.15	0.803731	0.8034 [25]	1.005[a]	140.84[b]	1223.17	1223.0 [25]	62.103
	298.15	0.799714	0.7995 [25]	1.007[a]	144.10 [26]	1206.47	1206.0 [25]	64.530
	303.15	0.795676	0.7955 [25] 0.79601 [27]	1.020[a]	147.36[b]	1189.86	1189.0 [25] 1189.0 [27]	67.066
	308.15	0.791602	0.79146 [28]	1.029[a]	150.62[b]	1172.04	1171.41 [28]	69.741
2-Propanol	293.15	0.785282	0.78507 [29]	1.055[a]	151.69[b]	1157.78	1156 [29]	72.701
	298.15	0.781073	0.780942 [24]	1.087[a]	158.8 [30]	1140.24	1139 [29]	75.765
	303.15	0.776790	0.776601 [24]	1.112[a]	159.91[b]	1122.59	1121 [29]	79.031
	308.15	0.772434	0.772559 [24]	1.128[a]	164.01 [30]	1104.51	1104.04 [31]	82.563
1-Butanol	293.15	0.809164	0.80917 [32]	0.902[a]	173.85[b]	1272.81	1257 [29] 1256.8 [33]	69.880
	298.15	0.8055704	0.80575 [29] 0.80554 [32]		177.10[b]	1255.81	1240 [29] 1239.8 [33]	72.426
	303.15	0.801899	0.80180 [29] 0.80190 [32]	0.907[a]	180.37[b]	1238.85	1224 [29] 1222.9 [33]	75.106
	308.15	0.798242	0.79825 [32]	0.916[a]	183.61[b]	1221.96	1206.2 [33]	77.906
2-Butanol	293.15	0.806854	0.80684 [29] 0.80657 [32]	1.004[a]	192.79[b]	1230.49	1230 [29] 1230.1 [33]	75.198
	298.15	0.802728	0.80228 [32]	1.039[a]	196.9 [34]	1212.54	1212 [29] 1212.1 [33]	78.239
	303.15	0.798513	0.79799 [32]	1.045[a]	201.02[b]	1194.48	1194 [29,33]	81.476
	308.15	0.794211	0.79372 [32]	1.083[a]	205.13[b]	1176.34	1175 [34]	84.921

[a] Derived from our measured densities.
[b] Calculated using group additivity.