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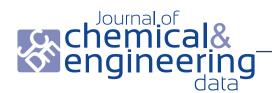


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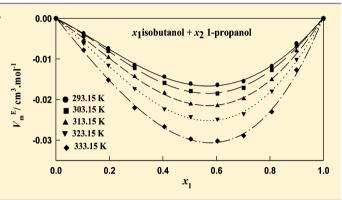
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1 Density and Viscosity Measurements of Binary Alkanol Mixtures ₂ from (293.15 to 333.15) K at Atmospheric Pressure

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ABSTRACT: Density and viscosity of binary mixtures of $\{x_1 \text{ isobutanol} + x_2 \text{ 1-propanol}\}, \{x_1 \text{ isobutanol} + x_2 \text{ 2-propanol}\},$ and $\{x_13\text{-amino-1-propanol} + x_21\text{-propanol}\}$ were measured over the entire composition range and from temperatures (293.15 to 333.15) K at ambient pressure. The excess molar volumes and viscosity deviations were calculated and correlated by the Redlich-Kister and McAllister equations, respectively. The excess molar volumes are negative over the entire mole fraction range for all of the mixtures and become more negative with increasing temperature. The viscosity deviations of the binary mixtures are negative in the entire composition range and decrease with increasing temperature.



17 INTRODUCTION

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18 Alkanols are important compounds in both industry and 19 science. Because the physiochemical properties of alkanols are 20 mainly affected by hydroxyl group, then these properties can 21 be used as input data for evaluating theoretical models related 22 to study the hydrophobic interactions. 2,3 Alkanols can also be 23 used in the synthesis of many other organic compounds. Some 24 industrial applications of alkanols consist of perfumes, 25 cosmetics, paint, varnish, drugs, fuel, explosives, fats, waxes, 26 resin, plastics, rubber, and detergents.

Amines, alkanols, and their binary mixtures have found 28 applications as solvent in chemistry and technology. 5 The 29 nature of interactions between amines and alcohols are 30 hydrogen bonding. Hydrogen bonding systems have important 31 roles in chemical, physical, and biological processes and drug 32 synthesis. 1,6 Aminoalcohols are an important class of organic 33 compounds which are used as chiral auxiliaries and ligands. 7-9 34 One member of these materials is 3-amino-1-propanol which 35 is used as an ice crystallization inhibitor 10 and for remov-36 ing acidic components carbon dioxide or hydrogen sulfide 37 from gas streams of industrial origin or from polluted 38 atmosphere. 11-13

Mixtures containing oxygenated compounds such as alkanols 40 are also important materials in the oil industry because of their 41 application in enhancing octane number in gasoline as additives 42 and pollution reducing properties. Binary mixtures of alkanols are 43 interesting due to their self-association between like molecules 44 and capability of forming intermolecular hydrogen bonds created 45 between unlike molecules upon mixing. So, the treatment of this 46 class of mixtures could be helpful in examination of theoretical

In this work, the excess molar volume, $V_{\rm m}^{\rm E}$, and viscosity deviation, 49 $\Delta\eta$, of some binary alkanol mixtures were presented. We have measu-50 red densities and viscosities of the binary mixtures {isobutanol + 51 1-propanol}, {isobutanol + 2-propanol}, and {3-amino-1-propanol +

1-propanol} along with their pure components in the temperature 52 range of (293.15 to 333.15) K. The data were measured over the 53 entire composition range at ambient pressure. For the studied 54 systems, we found no data in the literature. The obtained excess 55 molar volumes and viscosity deviations were correlated by 56 Redlich-Kister¹⁴ and McAllister¹⁵ equations, respectively. They 57 were also discussed via hydrogen bond interactions between 58 component molecules and packing effects, which origins from the 59 structural factors.

■ EXPERIMENTAL SECTION

Chemicals. Isobutanol and 3-amino-1-propanol were 62 supplied by Merck Company with purities higher than 99 %, 63 while 1-propanol was prepared by the same Company with 64 purity higher than 99.8 %. 2-Propanol was purchesed by BDH 65 with purity higher than 99.5 %. All the purities are in mass 66 fraction. The materials were degassed just before experiment 67 and have been used without further purification. The densities 68 and viscosities of pure components along with the literature 69 data¹⁶⁻³¹ are listed in Table 1.

Density Measurements. An Anton-Paar DMA 4500 71 model vibrating tube densimeter, was used for measuring 72 the densities of pure compounds and binary mixtures. The 73 accuracy in the determining density was estimated to be 74 $\pm 5.10^{-5}$ g·cm⁻³. The temperature in the cell was regulated to 75 ± 0.01 K with solid state thermostat. The apparatus was 76 calibrated once a day with dry air and double- distilled freshly 77 degassed water. ³² Air tight stopper bottles were used for the 78 preparation of the mixtures. The mass of dry bottle was first 79 determined. The less volatile component of the mixture was 80 introduced in the bottle, and the total mass was recorded. 81

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Table 1. Purities, Experimental Densities, and Viscosities along with Literature Data for Pure Compounds at Given Temperatures and Pressure of 0.1 MPa^a

		$ ho/{ m g}$	g·cm ^{−3}	η/mPa.·s		
purities in mass fraction	T/K	this work	lit.	this work	lit.	
		Isobut	anol			
99 %	293.15	0.80182	0.8018^{b}	4.087	4.033 ^c	
	303.15	0.79406	0.79406^d	2.877	2.876^{e}	
	313.15	0.78612	0.78612^d	2.091	2.080^{d}	
	323.15	0.77794	0.77793^d	1.576	1.602^{d}	
	333.15	0.76946	0.76944 ^d	1.125	1.116^{d}	
		3-Amino-1-	-propanol			
99 %	293.15	0.98765	0.98650 ^f	40.456		
	303.15	0.97965	0.9833^g	23.981	24.1204 ^g	
	313.15	0.97161	0.975191^h	15.312		
	323.15	0.96352	0.966881 ^h	10.221		
	333.15	0.95538		6.962		
		oanol				
99.8 %	293.15	0.80357	0.80359^{I}	2.204	2.204^{q}	
	303.15	0.79553	0.79553^{I}	1.513	1.6145^{k}	
	313.15	0.78735	0.78738^{I}	1.018	1.1883^{k}	
	323.15	0.77898	0.77892^{I}	0.790	0.8796^{k}	
	333.15	0.77038	0.77042^{1}	0.470	0.5985^{k}	
		2-Prop	anol			
99.5 %	293.15	0.78535	0.78535 ^j	2.362	2.362^{p}	
	303.15	0.77686	0.77680^{j}	1.762	1.763 ⁿ	
	313.15	0.76807	0.76800^{j}	1.200		
	323.15	0.75889	0.75890^{m}	0.938		
	333.15	0.74925	0.74920^{o}	0.604	0.624°	
					_	

^aStandard uncertainties u are $u(T) = \pm 0.01$ K, $u(\rho) = \pm 5 \cdot 10^{-5}$ g·cm⁻³, and $u(\eta) = \pm 5 \cdot 10^{-2}$ mPa·s. ^bReference 3. ^cReference 4. ^dReference 5. ^eReference 6. ^fReference 7. ^gReference 8. ^hReference 9. ^IReference 10. ^fReference 11. ^kReference 12. ^lReference 13. ^mReference 14. ⁿReference 15. ^oReference 16. ^pReference 17. ^qReference 18.

82 Subsequently, the other component was added, and the mass 83 of bottle including two components was determined. Each 84 mixture was immediately used, after it was mixed by shaking. 85 All the weightings were performed on an electronic digital 86 balance (AB 204-N Mettler) accurate to $\pm 1\cdot 10^{-5}$ g. The 87 possible error in the mole fraction is estimated to be lower 88 than $\pm 1\cdot 10^{-4}$. Conversion to molar quantities was based on 89 the relative atomic mass table of 2006 issued by IUPAC. 33 90 The uncertainty in the excess molar volumes estimated to 91 be $\pm 1\cdot 10^{-4}$ cm³. mol⁻¹.

Viscosity Measurements. Viscosity was determined using 92 an Ubbelohde viscometer which was fixed in a water bath and 93 the temperature was controlled with a precision of \pm 0.01 K. 94 The flow times were taken by using a digital chronometer 95 model of KENKO KK-5898 with a precision of \pm 0.01 s. 96

Measurements of density and viscosity were repeated at least 97 three times to get the best averaged values. 98

■ RESULTS AND DISCUSSION

Excess Molar Volume of Mixtures. The excess molar 100 volume of mixtures, $V_{m_l}^E$ can be calculated via the following equation: 101

$$V_{\rm m}^{\rm E} = V - \sum_{i=1}^{2} (x_i V_i^0) \tag{1}_{102}$$

where x_i and V_i^0 are the mole fraction and molar volume of the 103 pure component i at any temperature and V is the molar 104 volume of the mixture. The excess molar volumes can be 105 correlated via a polynomial presented by Redlich–Kister 4 as 106

$$V_{\rm m}^{\rm E} = x_1 x_2 \sum_{i=1}^{k} A_i (1 - 2x_1)^i$$
(2) 107

where x_1 and x_2 are the mole fractions of the components and k 108 is the order of polynomial equation (k = 4). A_i are the fitting 109 parameters that can be correlated in terms of temperature as 110

$$A_{i} = \sum_{j=0}^{2} B_{ij} T^{i}$$
(3) 111

The B_{ij} coefficients are mixture dependent parameters and T is 112 absolute temperature. These coefficients were calculated for $V_{\rm m}^{\rm E}$ 113 of binary mixtures and the results of such calculations are listed 114 in Table 2. The standard deviations reported in this table were 115 computed by using the following equation: 116

$$\sigma = \left(\sum_{i=1}^{n} \frac{(V_{\text{exp},i}^{\text{E}} - V_{\text{cal},i}^{\text{E}})^{2}}{(n-p)}\right)^{1/2}$$
(4) 117

where n is the number of experimental points and p is the 118 number of adjustable parameters, A_p in eq 2. Figure 1a—c 119 shows the negative excess molar volumes over the entire mole 120 fraction range for the binary mixtures under study that 121 become more negative with increasing temperature from 122 (293.15 to 333.15) K. These results are in consistency with 123 our previous results of {3-amino-1-propanol + isobutanol} 124 and {3-amino-1-propanol + 2-propane} mixtures. ³⁴ In all of 125

Table 2. Coefficients of Rerlich-Kister Equation, B_{ij} , and Standard Deviations in Excess Molar Volumes, $\sigma(V_{\rm m}^{\rm E})$, for Mixtures in the Temperature Range of (293.15 to 333.15) K

			i			
j	0	1	2	3	4	$\sigma(V_{\mathrm{m}}^{\mathrm{E}})/\mathrm{cm}^{3}\cdot\mathrm{mol}^{-1}$
0	-1.5312	-0.6434	-7.5174	3.6048	9.7855	
1	0.0106	0.0040	0.0488	-0.0233	-0.0633	0.0002
2	$1.9013 \cdot 10^{-5}$	$-5.7341 \cdot 10^{-6}$	$-7.9056 \cdot 10^{-5}$	$3.7468 \cdot 10^{-5}$	$1.0238 \cdot 10^{-4}$	
0	-1.5193	-2.0526	-2.0591	2.5554	2.7000	
1	0.0103	0.0127	0.0137	-0.0155	-0.0183	0.0003
2	$-1.8196 \cdot 10^{-5}$	$-1.9892 \cdot 10^{-5}$	$-2.2252 \cdot 10^{-5}$	$2.3914 \cdot 10^{-5}$	$3.0675 \cdot 10^{-5}$	
0	-9.0161	-2.3656	-12.9735	4.8957	17.8023	
1	0.0476	0.0156	0.0877	-0.0331	-0.1170	0.0039
2	$-8.6192 \cdot 10^{-5}$	$-2.5906 \cdot 10^{-5}$	$-1.5463 \cdot 10^{-4}$	$5.6650 \cdot 10^{-5}$	$1.9683 \cdot 10^{-4}$	

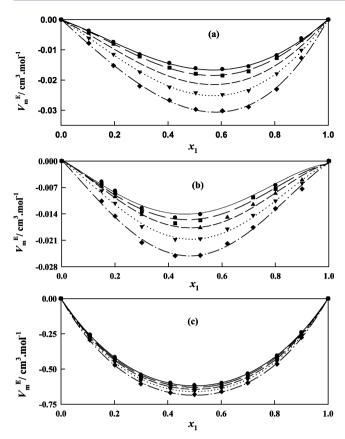


Figure 1. Excess molar volume, $V_{\rm m}^E$, versus mole fraction, x_1 , for (a) $\{x_1$ isobutanol + x_2 1-propanol $\}$, (b) $\{x_1$ isobutanol + x_2 2-propanol $\}$, and (c) $\{x_1$ 3-amino-1-propanol + x_2 1-propanol $\}$ at \bullet ,——, 293.15 K; \bullet ,——, 303.15 K; \bullet ,——, 313.15 K; \vee ,…, 323.15 K; \bullet ,—•—, 333.15 K. Solid lines and symbols indicate the calculated and experimental values, respectively.

126 the present and previous binary mixtures the excess molar 127 volumes are negative, which means that the interactions 128 between unlike molecules are stronger than those for like 129 molecules. Also, the magnitudes of negative values in excess 130 molar volumes in the mixtures containing 3-amino-1-propanol 131 are greater than other mixtures. In the mixture containing 3-132 amino-1-propanol with two functional groups of OH and 133 NH₂, the H-bond formation is more probable and so the 134 interactions are stronger than the other mixtures without such 135 an effectively associating fluid.

Viscosity of Binary Mixtures. The equation developed by McAllister has been used successfully to correlate viscosity data of binary mixtures. The equation contains two adjustable interaction parameters ν_{12} and ν_{21} . The importance of this model is that it may be considered as some kind of bridge between the transport and the thermodynamic properties. This model is widely recommended to provide theoretical values for viscosity close to the experimental data. The model is based on Eyring's theory of absolute reaction trates to present the kinematic viscosity of a binary mixture as

$$\ln \nu = x_1^3 \ln \nu_1 + x_2^3 \ln \nu_2 + 3x_1^2 x_2 \ln \nu_{12} + 3x_1 x_2^2 \ln \nu_{21}$$
$$- \ln \left(x_1 + x_2 \frac{M_2}{M_1} \right) + 3x_1^2 x_2 \ln \left(\frac{2 + M_2 / M_1}{3} \right)$$
$$+ 3x_1 x_2^2 \ln \left(\frac{1 + 2M_2 / M_1}{3} \right) + x_2^3 \ln \frac{M_2}{M_1}$$
(5)

The ν_{12} and ν_{21} are interaction parameters were obtained by 146 data regression, and $M_{\rm i}$ and ν_i are molecular mass and 147 kinematic viscosity of the pure component i, respectively. The 148 relation between the kinematic and dynamic viscosities is $\nu=149$ η/ρ . These calculations for the binary mixtures under study 150 were carried out using eq 5 and the experimental viscosities and 151 densities of a binary mixture over entire composition range 152 at any given temperature to find the η_{12} (= $\rho_{\rm mix}\nu_{12}$) and η_{21} 153 (= $\rho_{\rm mix}\nu_{21}$) parameters and the results are listed in Table 3. The 154 standard deviations reported in this table were computed by 155 using the following equation:

$$\sigma(\%) = \left(\frac{1}{n-k} \sum_{i=1}^{n} \sum_{i=1}^{n} \left\{ \frac{100(\eta_{\exp,i} - \eta_{\operatorname{cal},i})}{\eta_{\exp,i}} \right\}^{2} \right)^{1/2}$$
(6) 157

As Table 3 shows, the obtained viscosity interaction 158 parameters, η_{12} and η_{21} , for all of the mixtures under study 159 are positive values greater than unit. Then, the terms involving 160 them in eq 5 can increase viscosities of the mixtures. This table 161 also shows that the interaction parameters decrease with 162 increasing temperature, which is a reasonable result. It is well-163 known that viscosity of liquids decreases with increasing 164 temperature. These parameters also are greater in magnitude in 165 the case of {3-amino-1-propanol + 1-propane} mixture, which 166 is a mixture with stronger hydrogen bonds than the other 167 mixtures.

Using the obtained interaction parameters, the viscosity 169 deviations were obtained via the following relation:

$$\Delta \eta = \eta - (x_1 \eta_1 + x_2 \eta_2) \tag{7}$$

for the binary mixtures and applying eq 5. The results of such 172 calculations are listed in columns 4 and 5 of Table 4. As this 173

Table 3. Parameters of McAllister Equation and the Standard Deviations, $\sigma(\%)$, in Correlating the Viscosities of Mixtures in the Temperature Range of (293.15 to 333.15) K

	McAllister eq						
binary systems	T/K	$\eta_{12}/\text{mPa·s}$	$\eta_{21}/\text{mPa·s}$	$\sigma/\%$			
x_1 isobutanol + x_2 1-propanol	293.15	3.77	3.01	0.49			
	303.15	2.68	2.20	0.18			
	313.15	1.94	1.55	0.39			
	323.15	1.47	1.20	0.51			
	333.15	1.01	0.78	0.62			
x_1 isobutanol + x_2 2-propanol	293.15	4.21	3.14	0.11			
	303.15	3.01	2.31	0.23			
	313.15	2.17	1.64	0.52			
	323.15	1.66	1.30	0.58			
	333.15	1.17	0.90	0.58			
x_1 3-amino-1-propanol + x_2 1-propanol	293.15	22.91	7.67	0.15			
	303.15	14.02	4.91	1.07			
	313.15	9.37	4.01	2.95			
	323.15	7.11	2.75	0.16			
	333.15	5.32	1.50	0.15			

table shows, the relative viscosity deviations (calculated via 174 eq 7) are rarely more than 1. Figure 2a–c shows the obtained 175 viscosity deviations for the binary mixtures. As Figure 2 shows, 176 the viscosity deviations of all binary mixtures under study are 177 negative in the entire composition range and become less 178 negative with increasing temperature.

Table 4. Experimental Density, ρ , Excess Molar Volume, $V_{\rm m}^{\rm E}$, Viscosity, η , Viscosity Deviation, $\Delta\eta$, and Standard Deviation in the Viscosity, σ (%), for the Mixtures at Given Temperatures and Pressure of 0.1 MPa, over Entire Composition Range^a

$V_{\rm m}^{\rm E}/{\rm cm}^3\cdot{\rm mol}^{-1}$		Δη/mPa·s	σ/%
T/K = 30		Δη/IIII a·s	0/ /0
0.0061	1.817	-0.112	0.16
0.0085	1.839	-0.147	0.03
0.0133	1.907	-0.190	0.03
0.0165	2.021	-0.215	0.10
0.0157	2.131	-0.210	0.08
0.0122	2.271	-0.183	0.01
0.0096	2.417	-0.144	0.08
0.0074	2.547	-0.107	0.04
0.0045	2.709	-0.057	0.00
T/K = 31		0.037	0.00
-0.0068	1.259	-0.074	0.30
-0.0095	1.280	-0.098	0.19
-0.0142	1.331	-0.136	0.19
	1.418	-0.130 -0.160	0.07
-0.0185		-0.160 -0.157	0.20
-0.0177	1.505		
-0.0149	1.617	-0.136	0.00
-0.0115	1.732	-0.107	0.11
-0.0086	1.837	-0.076	0.15
-0.0050	1.963	-0.039	0.09
T/K = 32			
-0.0079	0.983	-0.050	0.29
-0.0112	0.999	-0.066	0.23
-0.0174	1.035	-0.094	0.05
-0.0208	1.095	-0.114	0.31
-0.0206	1.158	-0.111	0.20
-0.0180	1.237	-0.097	0.01
-0.0144	1.320	-0.075	0.15
-0.0106	1.394	-0.054	0.17
-0.0059	1.483	-0.030	0.07
T/K = 33	33.15		
-0.0106	0.648	-0.034	0.29
-0.0146	0.663	-0.046	0.19
-0.0216	0.696	-0.064	0.01
-0.0251	0.745	-0.080	0.31
-0.0250	0.794	-0.080	0.23
-0.0219	0.857	-0.070	0.00
-0.0176	0.921	-0.056	0.14
-0.0126	0.979	-0.041	0.16
-0.0074	1.051	-0.022	0.12
1-propanol + x_2 1-	i-Propanol T/	/K = 293.15	
-0.2568	2.978	-3.256	0.56
-0.4154	4.164	-5.644	0.19
-0.5405	5.873	-7.675	0.21
-0.5988	8.435	-9.361	0.06
-0.6145	11.256	-10.01	0.13
-0.5993	15.347	-9.805	0.30
-0.5323	20.076	-8.841	0.01
-0.4049	26.442	-6.686	0.33
-0.2401	32.707	-3.918	0.30
T/K = 30		5.710	0.50
-0.2638	2.081	-1.876	0.82
-0.2638 -0.4261	2.839	-3.210	0.82
-0.5510	3.890	-4.347	0.32
			0.25
			0.13
			0.23
-0.5421	12.288	-4.942	0.12
-0.4152			0.32
-0.2469	19.523	-2.217	0.33
	-0.4152	-0.6256 7.040 -0.6109 9.477 -0.5421 12.288 -0.4152 15.930	-0.6256 7.040 -5.711 -0.6109 9.477 -5.549 -0.5421 12.288 -4.942 -0.4152 15.930 -3.763

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Table 4. continued

x_1	$ ho/{ m g\cdot cm^{-3}}$	$V_{\rm m}^{\rm E}/{\rm cm}^3{ m \cdot mol}^{-1}$	$\eta/\text{mPa·s}$	$\Delta \eta / \text{mPa·s}$	$\sigma/\%$	x_1	$ ho/\mathrm{g}\cdot\mathrm{cm}^{-3}$	$V_{\rm m}^{\rm E}/{\rm cm}^3{\cdot}{\rm mol}^{-1}$	$\eta/\text{mPa·s}$	$\Delta \eta / \text{mPa·s}$	$\sigma/\%$
		T/K = 313	3.15					T/K = 323	3.15		
0.1088	0.81049	-0.2704	1.401	-1.172	2.67	0.6014	0.8978	-0.6371	4.685	-1.777	0.05
0.2019	0.82965	-0.4359	2.061	-1.843	0.14	0.6995	0.91521	-0.5724	5.816	-1.570	0.55
0.2993	0.84923	-0.5635	2.864	-2.431	0.81	0.8091	0.93393	-0.4443	7.232	-1.189	1.07
0.4099	0.87051	-0.6229	3.970	-2.907	0.61	0.9003	0.94849	-0.2631	8.570	-0.710	0.92
0.5002	0.88749	-0.6395	5.050	-3.118	0.12			T/K = 333	3.15		
0.6014	0.90608	-0.6235	6.590	-3.025	0.15	0.1088	0.79363	-0.2936	0.579	-0.598	5.09
0.6995	0.92340	-0.5561	8.276	-2.741	0.25	0.2019	0.81286	-0.4713	0.846	-0.935	1.69
0.8091	0.94203	-0.4277	10.504	-2.080	0.45	0.2993	0.83249	-0.6053	1.266	-1.147	1.60
0.9003	0.95659	-0.2542	12.627	-1.260	0.43	0.4099	0.85384	-0.6675	1.828	-1.303	2.08
		T/K = 323	3.15			0.5002	0.87085	-0.6811	2.352	-1.365	1.09
0.1088	0.80216	-0.2810	0.999	-0.817	4.67	0.6014	0.88948	-0.6596	3.105	-1.270	0.45
0.2019	0.82133	-0.4507	1.474	-1.220	0.85	0.6995	0.90701	-0.5984	3.907	-1.105	0.71
0.2993	0.84093	-0.5817	2.110	-1.503	1.43	0.8091	0.92577	-0.4643	4.917	-0.806	1.55
0.4099	0.86222	-0.6411	2.950	-1.705	1.86	0.9003	0.94036	-0.2760	5.829	-0.486	1.54
0.5002	0.87921	-0.6566	3.657	-1.851	0.57						

"Standard uncertainties u are $u(T) = \pm 0.01 \text{ K}$, $u(\rho) = \pm 5 \cdot 10^{-5} \text{ g} \cdot \text{cm}^{-3}$, $u(V_m^E) = \pm 1 \cdot 10^{-4} \text{ cm}^3 \cdot \text{mol}^{-1}$, and $u(\eta) = \pm 5 \cdot 10^{-2} \text{ mPa·s}$.

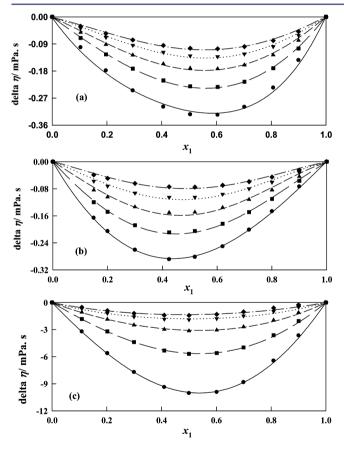


Figure 2. Viscosity deviations, $\Delta \eta$, versus mole fraction, x_1 , for (a) $\{x_1$ isobutanol + x_2 1-propanol $\}$, (b) $\{x_1$ isobutanol + x_2 2-propanol $\}$, and (c) $\{x_1$ 3-amino-1-propanol + x_2 1-propanol $\}$ at \bullet , — , 293.15 K; \bullet , — , 303.15 K; \bullet , — , 303.15 K; \bullet , — • , 333.15 K. Solid lines and symbols indicate the calculated and experimental values, respectively.

180 CONCLUSIONS

181 Density of binary mixtures of some binary mixtures of alkanols 182 were measured in the temperature range of (293.15 to 333.15) 183 K and over the entire composition range. The excess molar 184 volumes and viscosity deviations for the mixtures were calculated from experimental densities and viscosities data. 185 The obtained excess molar volumes are negative in the entire 186 composition range and become more negative by increasing the 187 temperature from (293.15 to 333.15) K. Increasing temperature 188 expands the volume of the mixture so that more spaces 189 between relative larger molecules will become available for the 190 relative smaller molecules to fill upon mixing. This effect will 191 pack the mixture volume.

The obtained viscosity deviations are negative over entire 193 composition range at all temperatures for all of the binary 194 mixtures, and become less negative with increasing temper- 195 ature. The attractive interactions between components of the 196 mixtures make weaker with increasing temperature and then 197 they can flow easer with lower viscosity.

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REFERENCES

- (1) Vijaya Krishna, T.; Madhu Mohan, T. Study of molecular 209 interactions in the polar binary mixtures of N-methyl aniline and 210 alcohols, using excess dielectric and thermodynamic parameters. *J.* 211 *Chem. Thermodyn.* **2012**, 47, 267–275.
- (2) Singh, S.; Parveen, S.; Shukla, D.; Gupta, M.; Shukla, J. P. 213 Volumetric, Optical, Acoustical and Viscometric Study of Molecular 214 Association in Binary Mixtures of Butylamine with 1- Butanol and 215 Tert-Butanol. *Acta Phys. Pol. A* **2007**, *6*, 847–858.
- (3) Bai, T. C.; Yao, J.; Han, S. J. Excess molar volumes for ternary 217 mixture *N*,*N*-dimethylform amide + 1-propanol + water at the 218 temperature 298.15 K Tong. *Fluid Phase Equilib.* **1998**, 152, 283–298. 219
- (4) Serbanovic, S. P.; Kijevcanin, M. L.; Radovic, I. R.; Djordjevic, B. 220 D. Effect of temperature on the excess molar volumes of some alcohol 221 + aromatic mixtures and modelling by cubic EOS mixing rules. *Fluid* 222 *Phase Equilib.* **2006**, 239, 69–82.
- (5) Iloukhani, H.; Khanlarzadeh, K. Volumetric properties for binary 224 and ternary systems consist of 1-chlorobutane, n-butylamine and 225

- 226 isobutanol at 298.15K with application of the Prigogine-Flory-227 Patterson theory and ERAS-Model. *Thermochim. Acta* **2010**, 502, 228 77–84.
- 229 (6) Dubey, G. P.; Kumar, K. Studies of thermophysical properties of 230 binary liquid mixtures of amine and alcohols at various temperatures. *J. 231 Chem. Thermodyn.* **2012**, *50*, 7–14.
- 232 (7) Uslu, A.; Kilic, A.; Guvenaltin, S. The investigation of structural 233 and thermosensitive properties of new phosphazene derivative bearing 234 glycol and aminoalcohol. *Inorg. Chem* **2010**, *363*, 3721–3726.
- 235 (8) Cacela, C.; Duarte, M. L.; Fausto, R. Structural and vibrational 236 characterisation of 3-amino-1-propanol a concerted SCF-MO ab initio, 237 Raman and infrared (matrix isolation and liquid phase) spectroscopy 238 study. *Spectrochim. Acta A* **2000**, *56*, 1051–1064.
- 239 (9) Emara, A. A. A.; Saleh, A. A.; Adly, O. M. I. Spectroscopic 240 investigations of new binuclear transition metal complexes of Schiff 241 bases derived from 4,6-diacetylresorcinol and 3-amino-1-propanol or 242 1,3-diamino-propane. *Spectrochim. Acta A* **2007**, *68*, 592–604.
- 243 (10) Cacela, C.; Baudot, A.; Duarte, M. L.; Matos-Beja, A. M.; Ramos 244 Silva, M.; Paixao, J. A.; Fausto, R. Low temperature polymorphism in 245 3-amino-1-propanol. *J. Mol. Struct.* **2003**, *649*, 143–153.
- 246 (11) Alvarez, E.; Cancela, A.; Maceiras, R.; Navaza, J. M.; Taboas, R. 247 Surface Tension of Aqueous Binary Mixtures of 1-Amino-2-Propanol 248 and 3-Amino-1-Propanol, and Aqueous Ternary Mixtures of These 249 Amines with Diethanolamine, Triethanolamine, and 2-Amino-2-250 methyl-1-propanol from (298.15 to 323.15) K. J. Chem. Eng. Data 251 2003, 48, 32–35.
- 252 (12) Henni, A.; Li, J.; Tontiwachwuthikul, P. Reaction Kinetics of 253 CO2 in Aqueous 1-Amino-2-Propanol, 3-Amino-1-Propanol, and 254 Dimethylmonoethanolamine Solutions in the Temperature Range of 255 298–313 K Using the Stopped-Flow Technique. *Ind. Eng. Chem. Res.* 256 **2008**, 47, 2213–2220.
- 257 (13) Dong, L.; Chen, J.; Gao, G. Solubility of Carbon Dioxide in 258 Aqueous Solutions of 3-Amino-1-propanol. *J. Chem. Eng. Data* **2010**, 259 55, 1030–1034.
- 260 (14) Redlich, O.; Kister, A. T. Algebraic representation of 261 Thermodynamic Properties and the Classification of Solutions. *Ind.* 262 Eng. Chem 1948, 40, 345–348.
- 263 (15) McAllister, R. A. The viscosity of liquid mixtures. *AIChE J.* 264 **1960**, *6*, 427–431.
- 265 (16) Lide, D. R. CRC Handbook of Chemistry and Physics; 87th ed.;266 Taylor and Francis: New York, 2007.
- 267 (17) Farhan, A. M.; Awwad, A. M. Densities, Viscosities, and Excess 268 Molar Enthalpies of 2-Pyrrolidone + Butanol Isomers at *T*= (293.15, 269 298.15, and 303.15) K. *J. Chem. Eng. Data* **2009**, *54*, 2095–2099.
- 270 (18) Baylaucq, A.; Watson, G.; ZebergMikkelsen, C.; Bazile, J. P.; 271 Boned, C. Dynamic Viscosity of the Binary System 1-Propanol +
- 272 Toluene As a Function of Temperature and Pressure. *J. Chem. Eng.* 273 *Data* **2009**, 54, 2715–2721.
- 274 (19) Ali, A.; Nain, A. K.; Lal, B.; Chand, D. Densities, viscosities, and 275 refractive indices of binary mixtures of benzene with isomeric butanols 276 at 30 °C. *Int. J. Thermophys.* **2004**, *25*, 1835–1847.
- 277 (20) Herba, H.; Czechowski, G.; Zywucki, B.; Stockhausen, M.; 278 Jadzyn, J. Excess molar volumes of binary mixtures of amino alcohols 279 with 1,4-dioxane. *J. Chem. Eng. Data* **1995**, *40*, 214–215.
- 280 (21) Omrani, A.; Rostami, A. A.; Mokhtary, M. Densities and 281 volumetric properties of 1,4- dioxane with ethanol, 3-methyl-1-butanol, 282 3-amino-1-propanol and 2-propanol binary mixtures at various 283 temperatures. *J. Mol. Liq.* **2010**, *157*, 18–24.
- 284 (22) Alvarez, E.; Cerdeira, F.; Gomez-Diaz, D.; Navaza, J. M. Density, 285 Speed of Sound, Isentropic Compressibility, and Excess Volume of 286 Binary Mixtures of 1-Amino-2-propanol or 3-Amino-1-propanol with
- 287 2-Amino-2-methyl-1-propanol, Diethanolamine, or Triethanol amine 288 from (293.15 to 323.15) K. J. Chem. Eng. Data 2010, 55, 2567–2575. 289 (23) Zarei, H. A.; Shahvarpour, S. Volumetric Properties of Binary
- 290 and Ternary Liquid Mixtures of 1-Propanol (1) + 2-Propanol (2) + 291 Water (3) at Different Temperatures and Ambient Pressure (81.5
- 292 kPa). J. Chem. Eng. Data 2008, 53, 1660–1668.
- 293 (24) Fong-Meng, P.; Chye-Eng, S.; Tjoon-Tow, T.; Ibrahim, M. H. 294 Densities and viscosities of aqueous solutions of 1-propanol and 2-

- propanol at temperatures from 293.15 to 333.15 K. J. Mol. Liq. 2007, 295 136, 71–78.
- (25) Kermanpour, F.; Sharifi, T. Thermodynamic study of binary 297 mixture of x_1 [C6mim][BF4] + x_2 1-propanol: Measurements and 298 molecular modeling. *Thermochim. Acta* **2012**, 527, 211–218.
- (26) Zarei, H. A.; Jalili, F. Densities and derived thermodynamic 300 properties of (2-ethoxyethanol + 1-propanol, or 2-propanol, or 1,2- 301 propandiol) at temperatures from T=(293.15 to 343.15) K. J. Chem. 302 Thermodyn. 2007, 39, 55–66.
- (27) Dubey, G. P.; Kumar, K. Thermodynamic properties of binary 304 liquid mixtures of diethyl enetriamine with alcohols at different 305 temperatures. *Thermochim. Acta* **2011**, *524*, 7–17.
- (28) Gonzalez, B.; Dominguez, A.; Tojo, J. Viscosities, densities and 307 speeds of sound of the binary systems: 2-propanol with octane, or 308 decane, or dodecane at T=(293.15, 298.15, and 303.15) K. J. Chem. 309 Thermodyn. 2003, 35, 939–953.
- (29) Kermanpour, F. The excess molar properties of $\{x_1[C_6mim]$ 311 [BF4] + x_2 2-propanol $\}$: Application of ERAS model. *J. Mol. Liq.* **2012**, 312 169, 156–162.
- (30) Kao, Y. C.; Tu, C. H. Densities, viscosities, refractive indices, 314 and surface tensions for binary and ternary mixtures of 2-propanol, 315 tetrahydropyran, and 2,2,4-trimethylpentane. *J. Chem. Thermodyn.* 316 **2011**, 43, 216–226.
- (31) Kumagai, A.; Yokoyama, C. Liquid Viscosity of Binary Mixtures 318 of Methanol with Ethanol and 1-Propanol from 273.15 to 333.15 K. 319 *Int. J. Thermophys.* **1998**, *19*, 3–13.
- (32) Paar, A. DMA 4500 Densimiter; *Instruction Handbook*; Graz: 321 Austria, 2002.
- (33) Wieser, M. E. Atomic Weights of the Elements 2005 (IUPAC 323 Technical Report). *Pure Appl. Chem.* 2006, 78, 2051–2066.
- (34) Kermanpour, F.; Niakan, H. Z. Experimental excess molar 325 properties of binary mixtures of (3-amino-1-propanol + isobutanol, 2- 326 propanol) at T = (293.15 to 333.15) K and modeling the excess molar 327 volume by Prigogine–Flory–Patterson theory. *J. Chem. Thermodyn.* 328 **2012**, 54, 10–19.
- (35) Bosse, D.; Bart, H. J. Viscosity Calculations on the Basis of 330 Eyring's Absolute Reaction Rate Theory and COSMOSPACE. *Ind.* 331 Eng. Chem. Res. **2005**, 44, 8428–8435.