Densities, Viscosities, and Volumetric Properties of Binary Mixtures of 1,2-Propanediol + 1-Heptanol or 1-Hexanol and 1,2-Ethanediol + 2-Butanol or 2-Propanol at T = (298.15, 303.15, and 308.15) K

Asma Verdian Doghaei, Abbas A. Rostami,* and Abdollah Omrani

Faculty of Chemistry, University of Mazandaran, P.O. Box 453, Babolsar, Iran

Densities and viscosities for 1,2-propanediol + 1-heptanol or 1-hexanol and 1,2-ethanediol + 2-butanol or 2-propanol were measured over the whole composition range at (298.15, 303.15, and 308.15) K and at atmospheric pressure. From the experimental data, the excess molar volume, V_m^E, partial molar volumes, $\bar{V}_{m,1}$ and $\bar{V}_{m,2}$, and excess partial molar volumes, $\bar{V}_{m,1}^E$ and $\bar{V}_{m,2}^E$, over the entire range of composition were calculated. Viscosity deviations, $\Delta\eta$, were also obtained and showed negative values for all investigated systems. These results were fitted to the Redlich−Kister polynomial equation to estimate the binary interaction parameters. The viscosity data were correlated with equations of McAllister, and calculated functions have been used to explain the intermolecular interaction between the mixing components.

Introduction

Hydrogen-bonded systems are very interesting because they play a vital role in chemical, physical, and biological processes.[1] It is well-known that alcohols are highly associated through hydrogen bonds, and this association decreases with the increase in molar mass of alkanols.[2] In recent years, measurements of thermodynamic and transport properties have been adequately employed in understanding the nature of molecular systems and physicochemical behavior in liquid mixtures.[3] Polyhydroxy compounds are used in a wide variety of end-use applications from cosmetics and household detergents to paints and automotive brake fluids. Alkanediols such as 1,2-propanediol are the simplest and model structural units for polyhydroxy compounds. These compounds play a significant role in industry due to their wide range of practical applications such as antifreezes, coolants, aircraft deicing fluids, heat transfer fluids, hydraulic fluids, solvents, food, flavor and fragrances, pharmaceuticals, chemical intermediates, plasticizers, thermoset plastic formulations, petroleum, textile, and other industries.[4] Volumetric properties of binary mixtures are complex properties because they depend not only on solute−solute, solvent−solvent, and solute−solvent interactions but also on the structural effect arising from interstitial accommodation due to the difference in volume and free volume between components present in the solution.[5] This properties have been extensively studied because the knowledge of these properties, including densities at different temperatures, is required for engineering design and subsequent operations. Moreover, there is interest in using volumetric data to test molecular theories or models of solution to extend our knowledge about molecular interactions between components.[6] A review of the literature shows that some thermophysical properties of the binary mixtures 1,2-ethanediol + 1-alkanol (C_1 to C_9 except C_7) and 1,2-propanediol + methanol, ethanol, 1-propanol, and 2-propanol have been reported,[1,7−10] but with regard to our mixtures, there are no experimental values. In the present paper, we report densities, ρ, of 1,2-propanediol + 1-heptanol or 1-hexanol and 1,2-ethanediol + 2-butanol or 2-propanol mixtures, including those of pure liquids at atmospheric pressure and temperatures of (298.15, 303.15, and 308.15) K, expressed by the mole fraction, x, of alkanol. The experimental values of ρ were used to calculate the excess molar volume, V_m^E, partial molar volumes, $\bar{V}_{m,1}$ and $\bar{V}_{m,2}$, and excess partial molar volumes, $\bar{V}_{m,1}^E$ and $\bar{V}_{m,2}^E$, over the whole composition range. The variation of these parameters with the composition and temperature of the mixtures have been discussed in terms of molecular interaction in these mixtures. The viscosity deviations, $\Delta\eta$, were also calculated from the experimental measurements. The viscosity data were correlated with the equation of McAllister.[11]

Experimental Section

Materials. 1,2-Propanediol, 1,2-ethanediol, 1-heptanol, 1-hexanol, and 2-propanol were purchased from Fluka, and 2-butanol was supplied by Merck with a purity higher than 99.7 %. All reagents were used without further purification. Binary mixtures were prepared by known masses of each liquid in airtight stoppered glass bottles.

Apparatus and Procedure. The mass measurements were made on a single pan Mettler balance with an accuracy of ± 0.01 mg. The possible error in mole fraction was calculated to be less than ± $1 \cdot 10^{-4}$. Density (ρ) measurements of pure components and binary mixtures over the complete composition range were carried out using a Anton Paar oscillating U-tube densitometer (model: DA 500) with ± 10^{-4} g·cm^{-3} accuracy. It was calibrated with double-distilled water and air. The temperature was regulated using a circulating bath (model: Heto DBT) with a precision of 0.01 K. The kinematic viscosity was measured with Ubbelohde viscometer with a Schott-Geräte automatic measuring unit (model: AVS 400) provided with a transparent thermostat, which allows temperature stabilization with a tolerance of 0.01 K. Different capillaries having various diameters were utilized depending on the sample viscosity. The kinematic viscosities were obtained using the following equation

$$\nu = kt \tag{1}$$

where k is the capillary constant of the viscosmeter and t is the flow time. The absolute viscosities, η, were calculated from η

* Corresponding author. E-mail address: rostami@umz.ac.ir. Tel.: +98-112-5342380. Fax: +98-112-5342350.

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Table 1. Pure Component Properties and Their Comparison with the Literature Values at 298.15 K

	ρ/g·cm^{-3}		η/mPa·s	
compound	exptl	lit.	exptl	lit.
1,2-propanediol	1.0331	1.0328[8]	45.440	
1,2-ethanediol	1.1092	1.1100[8]	15.408	16.1[11]
1-heptanol	0.8189	0.81888[9]	5.914	5.81[12]
1-hexanol	0.8154	0.81534[10]	4.643	4.59[8]
2-butanol	0.8024	0.80239[8]	2.999	2.998[12]
2-propanol	0.7820	0.78085[13]	2.037	2.04336[11]

Table 2. Viscosities, Densities, Excess Molar Volumes, and Partial Molar Volumes of 1-Heptanol (x_1) + 1,2-Propanediol (x_2) at T = (298.15, 303.15, and 308.15) K

x_1	ρ / g·cm^{-3}	η / mPa·s	V_m^E / cm^3·mol^{-1}	$\bar{V}_{m,1}$ / cm^3·mol^{-1}	$\bar{V}_{m,2}$ / cm^3·mol^{-1}
			T/K = 298.15		
0.0000	1.0331	45.440	0.000	143.070	73.662
0.1383	0.9803	27.341	0.188	143.180	73.673
0.3163	0.9288	15.902	0.345	142.550	73.863
0.3860	0.9125	13.641	0.359	142.380	73.942
0.4049	0.9083	13.192	0.368	142.352	73.969
0.4673	0.8954	11.941	0.369	142.256	74.038
0.6097	0.8697	9.882	0.348	142.087	74.253
0.7341	0.8510	8.159	0.262	141.924	74.566
0.8294	0.8385	7.132	0.165	141.856	74.820
1.0000	0.8189	5.914	0.000	141.895	73.798
			T/K = 303.15		
0.0000	1.0299	33.995	0.000	144.495	73.891
0.1383	0.9764	20.687	0.239	143.919	73.941
0.3163	0.9250	12.796	0.388	143.188	74.144
0.3860	0.9086	10.878	0.414	143.034	74.234
0.4049	0.9044	10.749	0.424	143.006	74.262
0.4673	0.8916	9.431	0.414	142.897	74.326
0.6097	0.8660	7.655	0.381	142.703	74.561
0.7341	0.8473	6.401	0.296	142.543	74.903
0.8294	0.8349	5.815	0.187	142.470	75.146
1.0000	0.8154	5.045	0.000	142.507	74.208
			T/K = 308.15		
0.0000	1.0254	26.338	0.000	145.483	74.215
0.1383	0.9720	16.050	0.253	144.534	74.282
0.3163	0.9208	9.977	0.410	143.842	74.481
0.386	0.9046	8.925	0.424	143.666	74.563
0.4049	0.9004	8.567	0.435	143.635	74.597
0.4673	0.8876	7.663	0.434	143.513	74.685
0.6097	0.8622	6.373	0.392	143.292	74.952
0.7341	0.8437	5.414	0.290	143.147	75.232
0.8294	0.8313	4.963	0.186	143.101	75.402
1.0000	0.8119	4.340	0.000	143.121	74.886

$= \rho\nu$. The viscosities were averaged from four readings. The accuracy in the viscosity measurement was ± 0.001 mPa·s.

Results and Discussion

The reliability of experimental measurements of ρ was ascertained by comparing the experimental data of pure liquids with the corresponding values which were available in the literature[12−17] at the studied temperatures. This comparison was given in Table 1, and agreement between the experimental and the literature values can be observed as well.

Measured densities, ρ, viscosities, η, excess molar volume, V_m^E, and partial molar volumes, $\bar{V}_{m,1}$ and $\bar{V}_{m,2}$, for the binary systems of 1,2-propanediol + 1-heptanol or 1-hexanol and 1,2-ethanediol + 2-butanol or 2-propanol at (298.15, 303.15, and 308.15) K at atmospheric pressure were given in Tables 2 to 5, respectively. The excess molar volume, V_m^E, and viscosity deviation, $\Delta\eta$, were calculated through the following equations

$$V^E/(\mathrm{cm^3 \cdot mol^{-1}}) = \sum_{i=1}^{n} x_i M_i \left(\frac{1}{\rho} - \frac{1}{\rho_i}\right) \quad (2)$$

$$\Delta\eta = \eta - \sum_{i=1}^{n} (x_i \eta_i) \quad (3)$$

where, for each equation, x, M, ρ, η, and V are the mole fraction, molar mass, density, dynamic viscosity, and molar volume, respectively. The subscript i represents the pure components. Composition dependences of the excess molar volume, V_m^E, and viscosity deviation, $\Delta\eta$, were represented by a Redlich−Kister type of equation[18]

$$Y = x(1 - x) \sum_{i=0}^{n} A_i (2x - 1)^i \quad (4)$$

where Y is V_m^E or $\Delta\eta$ and x refers to the mole fractions of the alkanols. In each case, an optimum number of coefficients was ascertained from an examination of the variation in standard deviation, σ, as given by

$$\sigma(Y) = [\sum (Y_{calcd} - Y_{exptl})^2/(N - n)]^{1/2} \quad (5)$$

where N is number of data points and n is the order of the fitting polynomial. The coefficients A_i for all of the mixtures calculated and results are given in Table 6 along with their standard deviations. Results presented in Tables 2 to 5 and Figure 1 indicate that V_m^E values are negative for (1,2-ethanediol +

Table 3. Viscosities, Densities, Excess Molar Volumes, and Partial Molar Volumes of 1-Hexanol (x_1) + 1,2-Propanediol (x_2) at T = (298.15, 303.15, and 308.15) K

x_1	ρ / g·cm^{-3}	η / mPa·s	V_m^E / cm^3·mol^{-1}	$\bar{V}_{m,1}$ / cm^3·mol^{-1}	$\bar{V}_{m,2}$ / cm^3·mol^{-1}
			T/K = 298.15		
0.0000	1.0331	45.440	0.000	127.326	73.662
0.0771	1.0045	33.270	0.117	126.413	73.696
0.1213	0.9899	28.443	0.145	126.181	73.707
0.2425	0.9536	18.556	0.247	126.010	73.765
0.3311	0.9307	14.378	0.281	125.900	73.791
0.5225	0.8887	9.486	0.315	125.548	74.064
0.5377	0.8857	9.057	0.319	125.529	74.101
0.6309	0.8689	7.625	0.270	125.397	74.250
0.7444	0.8503	6.313	0.219	125.368	74.358
0.8611	0.8333	5.324	0.135	125.354	74.379
1.0000	0.8154	4.643	0.000	125.313	75.273
			T/K = 303.15		
0.0000	1.0299	33.994	0.000	128.423	73.891
0.0771	1.0009	24.281	0.139	127.155	73.937
0.1213	0.9862	20.822	0.171	126.821	73.961
0.2425	0.9499	13.934	0.264	126.563	74.032
0.3311	0.9270	11.277	0.292	126.470	74.052
0.5225	0.8849	8.063	0.324	126.164	74.297
0.5377	0.8819	7.837	0.328	126.146	74.332
0.6309	0.8651	6.725	0.273	126.007	74.475
0.7444	0.8464	5.206	0.230	125.978	74.605
0.8611	0.8294	4.610	0.141	125.957	74.644
1.0000	0.8115	3.998	0.000	125.915	75.551
			T/K = 308.15		
0.0000	1.0254	26.338	0.000	129.950	74.215
0.0771	0.9961	20.052	0.177	127.760	74.294
0.1213	0.9816	17.274	0.203	127.220	74.334
0.2425	0.9458	11.972	0.274	126.936	74.410
0.3311	0.9231	9.627	0.296	126.949	74.393
0.5225	0.8813	6.428	0.335	126.702	74.600
0.5377	0.8782	6.308	0.329	126.670	74.628
0.6309	0.8615	5.322	0.286	126.523	74.804
0.7444	0.8429	4.494	0.244	126.493	74.938
0.8611	0.8260	3.935	0.156	126.475	74.958
1.0000	0.8083	3.471	0.000	126.413	76.300

Table 4. Viscosities, Densities, Excess Molar Volumes, and Partial Molar Volumes of 2-Butanol (x_1) + 1,2-Ethanediol (x_2) at T = (298.15, 303.15, and 308.15) K

x_1	ρ / g·cm^{-3}	η / mPa·s	V_m^E / cm^3·mol^{-1}	$\bar{V}_{m,1}$ / cm^3·mol^{-1}	$\bar{V}_{m,2}$ / cm^3·mol^{-1}
			T/K = 298.15		
0.0000	1.1092	15.408	0.000	89.766	55.957
0.0514	1.0858	14.670	−0.095	90.293	55.970
0.1049	1.0627	13.781	−0.182	90.738	55.946
0.1847	1.0296	12.295	−0.238	91.270	55.916
0.2610	1.0003	10.824	−0.268	91.604	55.866
0.3516	0.9683	9.089	−0.285	91.828	55.813
0.4562	0.9345	7.352	−0.268	91.958	55.812
0.5039	0.9203	6.670	−0.265	91.981	55.821
0.6639	0.8769	4.971	−0.228	92.065	55.887
0.7723	0.8509	4.301	−0.198	92.154	55.829
0.8751	0.8282	3.790	−0.147	92.263	55.550
1.0000	0.8024	2.999	0.000	92.373	54.703
			T/K = 303.15		
0.0000	1.1042	12.731	0.000	89.288	56.211
0.0514	1.0818	12.196	−0.144	90.520	56.182
0.1049	1.0591	11.571	−0.251	91.349	56.101
0.1847	1.0259	10.428	−0.298	92.086	56.007
0.2610	0.9967	9.184	−0.331	92.404	55.903
0.3516	0.9646	7.756	−0.337	92.564	55.819
0.4562	0.9307	6.211	−0.306	92.634	55.788
0.5039	0.9164	5.641	−0.291	92.641	55.786
0.6639	0.8731	4.182	−0.249	92.627	55.813
0.7723	0.8473	3.618	−0.230	92.635	55.762
0.8751	0.8247	3.180	−0.181	92.709	55.404
1.0000	0.7987	2.499	0.000	92.801	53.689
			T/K = 308.15		
0.0000	1.1006	10.661	0.000	89.308	56.395
0.0514	1.0785	10.241	−0.171	90.715	56.359
0.1049	1.0556	9.795	−0.277	91.678	56.284
0.1847	1.0228	8.898	−0.364	92.489	56.149
0.2610	0.9934	7.897	−0.399	92.861	56.035
0.3516	0.9609	6.681	−0.393	93.067	55.954
0.4562	0.9269	5.441	−0.370	93.155	55.898
0.5039	0.9125	4.959	−0.353	93.171	55.888
0.6639	0.8689	3.803	−0.304	93.172	55.890
0.7723	0.8429	3.347	−0.275	93.186	55.823
0.8751	0.8201	3.034	−0.211	93.271	55.421
1.0000	0.7938	2.475	0.000	93.374	53.491

Table 5. Viscosities, Densities, Excess Molar Volumes, and Partial Molar Volumes of 2-Propanol (x_1) + 1,2-Ethanediol (x_2) at T = (298.15, 303.15, and 308.15) K

x_1	ρ / g·cm^{-3}	η / mPa·s	V_m^E / cm^3·mol^{-1}	$\bar{V}_{m,1}$ / cm^3·mol^{-1}	$\bar{V}_{m,2}$ / cm^3·mol^{-1}
			T/K = 298.15		
0.0000	1.1092	15.408	0.000	74.411	55.957
0.1306	1.0584	12.567	−0.286	75.078	55.894
0.2043	1.0305	11.074	−0.385	75.652	55.780
0.3062	0.9928	9.151	−0.444	76.200	55.602
0.4100	0.9563	7.443	−0.464	76.409	55.476
0.5067	0.9240	6.038	−0.451	76.450	55.445
0.5267	0.9176	5.768	−0.451	76.454	55.441
0.5957	0.8959	4.990	−0.434	76.490	55.410
0.7049	0.8633	3.870	−0.398	76.610	55.174
0.7051	0.8632	3.906	−0.394	76.614	55.177
0.8146	0.8321	3.032	−0.314	76.762	54.633
0.8680	0.8171	2.741	−0.225	76.831	54.354
1.0000	0.7820	2.037	0.000	76.846	54.438
			T/K = 303.15		
0.0000	1.1042	12.731	0.000	73.845	56.211
0.1306	1.0548	10.501	−0.370	75.173	56.102
0.2043	1.0271	9.289	−0.486	75.922	55.959
0.3062	0.9894	7.713	−0.553	76.600	55.733
0.4100	0.9526	6.261	−0.559	76.884	55.567
0.5067	0.9201	5.120	−0.537	76.948	55.508
0.5267	0.9136	4.908	−0.530	76.952	55.502
0.5957	0.8918	4.242	−0.506	76.973	55.472
0.7049	0.8590	3.347	−0.455	77.062	55.289
0.7051	0.8589	3.344	−0.452	77.065	55.290
0.8146	0.8278	2.694	−0.370	77.195	54.765
0.8680	0.8128	2.405	−0.279	77.272	54.416
1.0000	0.7772	1.763	0.000	77.321	53.631
			T/K = 308.15		
0.0000	1.1006	10.661	0.000	74.044	56.395
0.1306	1.0513	8.954	−0.385	75.483	56.286
0.2043	1.0236	7.946	−0.507	76.248	56.134
0.3062	0.9858	6.553	−0.573	76.935	55.911
0.4100	0.9490	5.322	−0.584	77.208	55.755
0.5067	0.9166	4.335	−0.571	77.267	55.655
0.5267	0.9100	4.157	−0.558	77.281	55.645
0.5957	0.8881	3.574	−0.528	77.324	55.659
0.7049	0.8553	2.836	−0.479	77.442	55.414
0.7051	0.8552	2.819	−0.475	77.446	55.417
0.8146	0.8239	2.282	−0.376	77.601	54.850
0.8680	0.8088	2.076	−0.275	77.678	54.531
1.0000	0.7733	1.531	0.000	77.711	54.285

2-butanol or 2-propanol) and are positive for (1,2-propanediol + 1-heptanol or 1-hexanol) mixtures over the entire mole fraction range and at all temperatures investigated for each binary system under study. The observed negative V_m^E values for (1,2-ethanediol + 2-butanol or 2-propanol) mixtures are due to the formation of hydrogen bonding between unlike molecules resulting in a decrease in the volume of mixture. Another negative contribution to V_m^E comes from the structural contributions that arise from the geometrical fitting of one component into other owing to differences in molar volumes and free volumes between the components.[19] The positive V_m^E values indicate a loose packing of molecules in the mixtures, that is, a dilatation. Most likely, in this case different molecular sizes and shapes of propylene glycol, 1-heptanol, and 1-hexanol lead to interstitial accommodation in the mixtures. Simultaneously, it seems that the disruption of hydrogen-bonded structures upon mixing should be also taken into account.[1] A comparison of our results for V_m^E at T = 298.15 K with those reported for 1,2-ethanediol + alkanol shows that the V_m^E values for 1,2-ethanediol + alkanol for a given x decreases at T = 298.15 K in the sequence 2-butanol > 2-propanol. The V_m^E values for (1,2-propanediol + 1-alkanol) for a given x decrease at T = 298.15 K in the sequence 1-heptanol > 1-hexanol. It was observed that the magnitude of V_m^E depends upon the chain length in these alkanol molecules. The V_m^E values decrease (become more negative) for the 1,2-ethanediol + 2-butanol or 2-propanol systems, while its values increase (become more positive) for the binary mixtures having 1,2-propanediol with the temperature increased (see Tables 2 to 5).

We have also calculated partial molar volumes, $\bar{V}_{m,1}$ of component 1 (alkanol) and $\bar{V}_{m,2}$ of component 2 (alkandiol) in these mixtures by using the following relations[20]

$$\bar{V}_{m,1} = V_m^E + V_{m,1}^* + (1 - x)(\partial V_m^E/\partial x)_{T,P} \quad (6)$$

$$\bar{V}_{m,2} = V_m^E + V_{m,2}^* - x(\partial V_m^E/\partial x)_{T,P} \quad (7)$$

where $V_{m,1}^*$ and $V_{m,2}^*$ are the molar volumes of pure components alkanol and alkandiol, respectively. The derivative term, $(\delta V_m^E/\delta x)_{T,P}$, in eqs 6 and 7 was obtained by differentiation of eq 4, which leads to the following equations for $\bar{V}_{m,1}$ and $\bar{V}_{m,2}$

$$\bar{V}_{m,1} = V_{m,1}^* + (1 - x)^2 \sum_{i=0}^{n} A_i(1 - 2x)^i + 2x(1 - x)^2 \sum_{i=0}^{n} A_i(1 - 2x)^{i-1} \quad (8)$$

$$\bar{V}_{m,2} = V^*_{m,2} + x^2 \sum_{i=0}^{n} A_i(1 - 2x)^i + 2x^2(1 - x) \sum_{i=0}^{n} A_i(1 - 2x)^{i-1} \quad (9)$$

The excess partial molar volumes, $\bar{V}^E_{m,1}$ and $\bar{V}^E_{m,2}$, were then calculated by using the following relations

$$\bar{V}^E_{m,1} = \bar{V}_{m,1} - V^*_{m,1} \quad (10)$$

$$\bar{V}^E_{m,2} = \bar{V}_{m,2} - V^*_{m,2} \quad (11)$$

The variation in excess partial molar volumes $\bar{V}^E_{m,1}$ and $\bar{V}^E_{m,2}$ with composition at 298.15 K was presented in Figures 2 and 3, respectively. A close perusal of Figures 2 and 3 indicates that the values of $\bar{V}^E_{m,1}$ and $\bar{V}^E_{m,2}$ are negative for the 1,2-ethanediol + 2-butanol or 2-propanol binary mixtures. The values of $\bar{V}^E_{m,1}$ and $\bar{V}^E_{m,2}$ are positive over the whole composition range for 1,2-propanediol + 1-heptanol or 1-hexanol mixtures. These forms of variations further support the trends observed in V^E_m values for the binary systems examined here.

Table 6. Coefficients of the Redlich−Kister Equation and Their Standard Deviations

	A_0	A_1	A_2	A_3	A_4	σ
1,2-Propanediol + 1-Heptanol						
T/K = 298.15						
V^E	1.478	−0.191	0.250	−0.328	−1.072	0.004
$\Delta\eta$	−57.080	47.291	−35.395	−0.821	−12.851	0.043
T/K = 303.15						
V^E	1.663	−0.266	0.291	−0.570	−0.801	0.005
$\Delta\eta$	−42.143	28.335	−20.304	11.090	−2.158	0.108
T/K = 308.15						
V^E	1.721	−0.375	0.043	−0.470	−0.248	0.004
$\Delta\eta$	−31.746	22.748	−20.691	8.875	5.754	0.080
1,2-Propanediol + 1-Hexanol						
T/K = 298.15						
V^E	−1.280	−0.166	−0.605	−0.035	1.137	0.009
$\Delta\eta$	−61.254	42.337	−24.465	10.746	−8.981	0.155
T/K = 303.15						
V^E	1.334	−0.156	−0.458	−0.267	1.235	0.010
$\Delta\eta$	−42.951	33.157	−24.452	4.305	−22.866	0.150
T/K = 308.15						
V^E	−1.334	−0.022	−0.541	−0.703	2.018	0.011
$\Delta\eta$	−32.633	20.248	−15.342	7.015	2.647	0.030
1,2-Ethanediol + 2-Butanol						
T/K = 298.15						
V^E	−1.043	0.381	−0.960	−0.150	0.073	0.006
$\Delta\eta$	−9.947	−2.360	8.346	0.710	−0.655	0.007
T/K = 303.15						
V^E	−1.176	0.530	−1.149	−0.035	−0.692	0.008
$\Delta\eta$	−7.810	−3.219	9.562	0.979	−3.3013	0.020
T/K = 308.15						
V^E	−1.428	0.605	−1.238	−0.024	−0.818	0.003
$\Delta\eta$	−6.401	−3.173	9.447	1.362	−4.440	0.028
1,2-Ethanediol + 2-Propanol						
T/K = 298.15						
V^E	−1.803	0.225	−1.609	0.233	1.435	0.006
$\Delta\eta$	−10.333	−0.028	1.140	0.406	0.796	0.022
T/K = 303.15						
V^E	−2.143	0.560	−1.880	−0.067	1.041	0.005
$\Delta\eta$	−8.222	−0.218	2.245	0.427	−0.035	0.009
T/K = 308.15						
V^E	−2.254	0.501	−1.894	0.263	1.275	0.007
$\Delta\eta$	−6.796	−0.817	2.245	−0.086	1.473	0.011

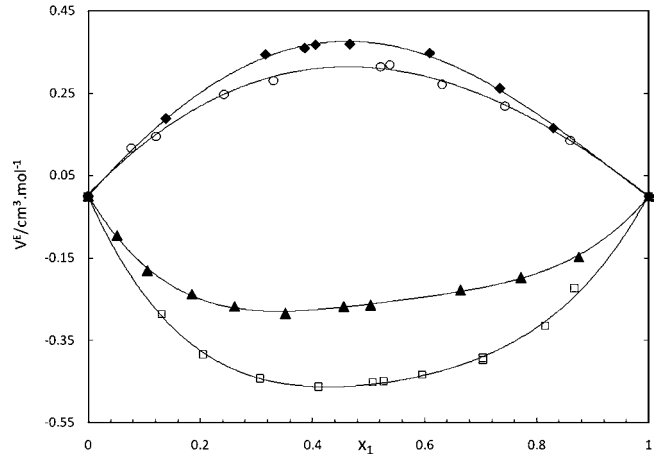

Figure 1. Dependence of excess molar volumes, V^E, as a function of mole fraction of alkanols for binary mixtures at 298.15 K. ◆, 1-heptanol (x_1) + 1,2-propanediol (x_2); ○, 1-hexanol (x_1) + 1,2-propanediol (x_2); ▼, 2-butanol (x_1) + 1,2-ethanediol (x_2); □, 2-propanol (x_1) + 1,2-ethanediol (x_2).

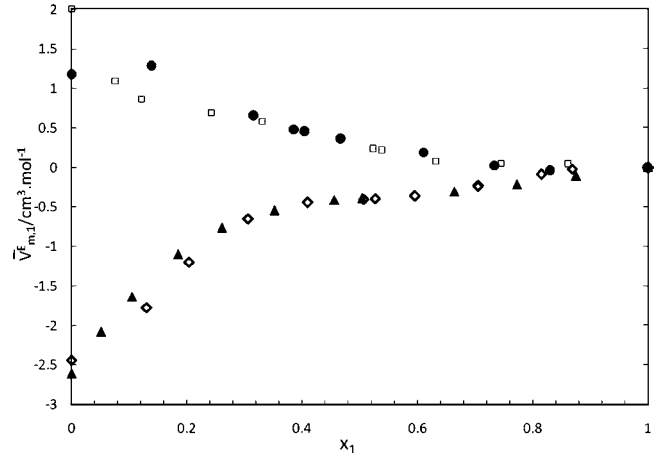

Figure 2. Excess partial molar volumes, $\bar{V}^E_{m,1}$, for the binary mixtures at 298.15 K. ●, 1-heptanol (x_1) + 1,2-propanediol (x_2); □, 1-hexanol (x_1) + 1,2-propanediol (x_2); ▼, 2-butanol (x_1) + 1,2-ethanediol (x_2); ◇, 2-propanol (x_1) + 1,2-ethanediol (x_2).

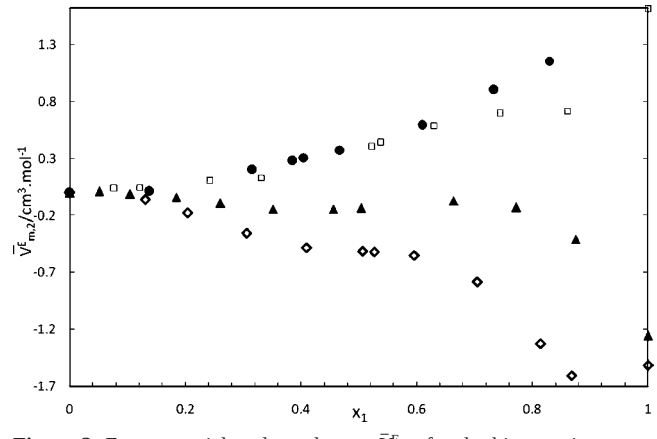

Figure 3. Excess partial molar volumes, $\bar{V}^E_{m,2}$, for the binary mixtures at 298.15 K. ●, 1-heptanol (x_1) + 1,2-propanediol (x_2); □, 1-hexanol (x_1) + 1,2-propanediol (x_2); ▲, 2-butanol (x_1) + 1,2-ethanediol (x_2); ◇, 2-propanol (x_1) + 1,2-ethanediol (x_2).

Several semiempirical relations have been proposed to estimate the dynamic viscosity of liquid mixtures in terms of pure-component data.[21] That refers to the equations of Kendall and Monroe,[22] Grunberg and Nissan,[23] Hind et al.,[24] Katti and Chaudhri,[25] McAllister,[11] Heric and Brewer,[26] and Auslaender.[27]

Table 7. Interactions Parameters of the McAllister Equation and Their Standard Deviations

composition	*T*/K	ν_{12}	ν_{21}	σ
1,2-ethanediol + 2-butanol	298.15	4.983	11.321	0.026
	303.15	4.162	9.954	0.028
	308.15	3.684	8.608	0.029
1,2-ethanediol + 2-propanol	298.15	4.726	9.845	0.005
	303.15	4.372	8.196	0.009
	308.15	3.414	7.347	0.012
1,2-propanediol + 1-heptanol	298.15	10.957	11.909	0.020
	303.15	7.898	10.378	0.011
	308.15	6.917	7.983	0.012
1,2-propanediol + 1-hexanol	298.15	7.789	13.347	0.012
	303.15	7.226	10.309	0.075
	308.15	5.688	9.374	0.007

From among various other existing equations used for the prediction of mixture viscosities, we have examined the equation proposed by McAllister for the evaluation of kinematic viscosity because it was shown that this model is quite sufficient for the alkanol binary systems.[28,29] The two-parameter McAllister equation was used as

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

where ν_{12} and ν_{21} are two three-body interaction parameters. The results are summarized in Table 7, where the parameters ν_{12} and ν_{21} and their standard deviations are given.

Figures 4 and 5 show that the viscosity deviation for all of the investigated systems is negative. Negative viscosity deviations from rectilinear dependence on mole fraction may also occur where dispersion forces are dominant, particularly for the system having different molecular sizes.[30]

Conclusion

The experimental data of densities and viscosities of 1,2-propanediol + 1-heptanol or 1-hexanol and 1,2-ethanediol + 2-butanol or 2-propanol were measured over the entire composition range and several temperatures. These data have been used to compute excess properties of the systems, and a Redlich−Kister type equation was used for fitting each set of excess properties. Also, our results showed that excess molar volume for the systems having ethylene glycol were negative, while those values for propylene glycol were found to be positive. The deviations in viscosity were negative for all of the systems examined here. Furthermore, it was observed that the values of excess properties are dependent on temperature. Also, we have calculated excess partial molar volumes and partial molar volumes of each component. The viscosity data were correlated with the equations of McAllister.

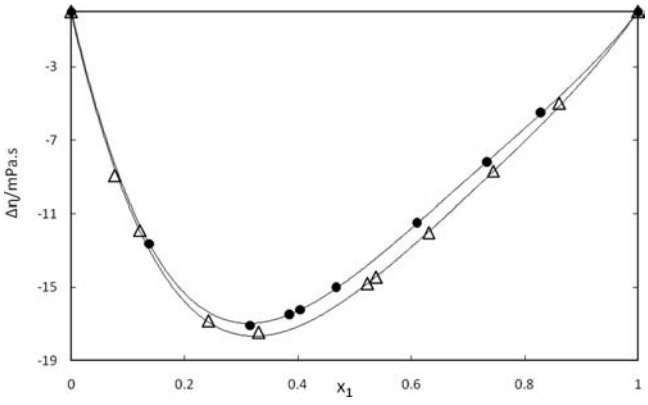

Figure 4. Dependence of viscosity deviations, $\Delta\eta$, as a function of mole fraction of alkanols for binary mixtures at 298.15 K. ●, 1-heptanol (x_1) + 1,2-propanediol (x_2); △, 1-hexanol (x_1) + 1,2-propanediol (x_2).

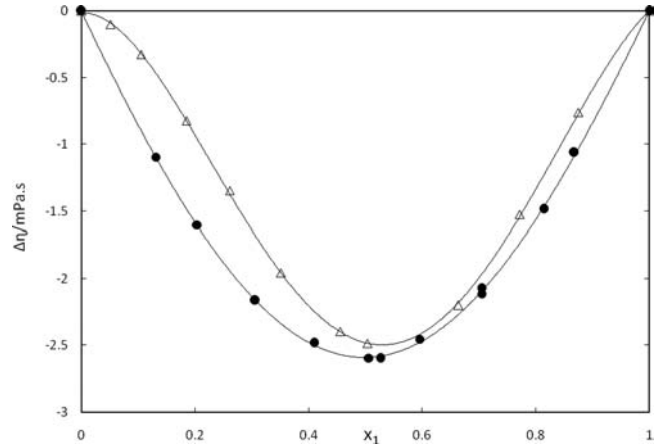

Figure 5. Dependence of viscosity deviations, $\Delta\eta$, as function of mole fraction of alkanols for binary mixtures at 298.15 K. △, 2-butanol (x_1) + 1,2-ethanediol (x_2); ●, 2-propanol (x_1) + 1,2-ethanediol (x_2).

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