JOURNAL OF CHEMICAL & ENGINEERING DATA

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Densities, Viscosities, Refractive Indexes, and Surface Tensions for Mixtures of Ethanol, Benzyl Acetate, and Benzyl Alcohol

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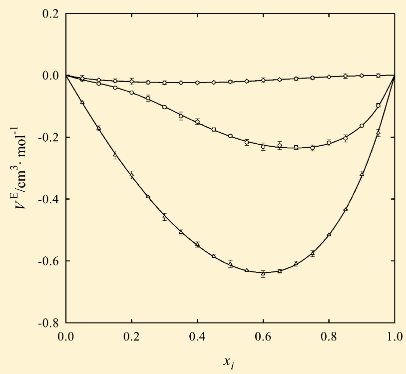
ABSTRACT: Densities, viscosities, refractive indexes, and surface tensions of the ternary system (ethanol + benzyl acetate + benzyl alcohol) at T = 303.15 K and its constituent binary systems (ethanol + benzyl acetate, ethanol + benzyl alcohol, and benzyl acetate + benzyl alcohol) at T = (293.15, 303.15, 313.15, and 323.15) K were measured under atmospheric pressure. Densities were determined using a vibrating-tube densimeter. Viscosities were measured with an automatic microviscometer based on the rolling-ball principle. Refractive indexes were measured using a digital Abbe-type refractometer. Surface tensions were determined by the Wilhelmy-plate method. From these data, excess molar volumes, deviations in viscosity, deviations in refractive index, and deviations in surface tension were derived. The results for the binary and ternary systems were fitted to the Redlich−Kister equation and the Cilbuka equation, respectively. The excess molar volumes and deviations in viscosity are used to study the nature of mixing behaviors between mixture components.



■ INTRODUCTION

The flavor compounds are vitally interrelated to our daily lives. This paper is concerned with the measurement of the mixing properties for two kinds of flavor compounds, such as benzyl acetate and benzyl alcohol, mixed with ethanol. Benzyl alcohol was chosen for the present study because, except for its usage in perfumery and oral cavity sanitation as an antimicrobial agent, it is widely used in microscopy as the embedding material.[1] Benzyl alcohol is also important as a solvent for gelatin, cellulose acetate, and shellac.[2] Benzyl acetate has found its usage in artificial essences and as a base solvent for some flavor compounds. Ethanol is a versatile solvent with protic and self-associated properties, which can be used to study hydrophobic effects.

In this work, the effects of composition and temperature upon densities (ρ), viscosities (η), refractive indexes (n_D), and surface tensions (σ) for the systems formed by ethanol, benzyl acetate, and benzyl alcohol have been analyzed. More specifically, smooth representations of the excess molar volumes (V^E) are described. This kind of study is important toward the understanding of the molecular interaction between mixture components. In our previous papers, experimental densities, viscosities, refractive indexes, and surface tensions for ethanol + benzyl acetate were reported at T = (288.15, 298.15, 308.15, and 318.15) K.[3,4] However, we are not aware of any literature data regarding the properties for the mixtures presented in this study.

■ EXPERIMENTAL SECTION

Materials. The chemicals used were of analytical grade and supplied by Merck (Germany). The pure components were stored over 0.3 nm molecular sieve to prevent water absorption. They were used without any further purification. The amount of water in each pure sample was monitored along the time it took to carry out the present study with a Karl Fischer V20 moisture meter, Mettler. The purity of all chemicals was checked using a Perkin-Elmer Autosystem gas chromatograph (GC). The sources, purities, and analysis methods of the chemicals are shown in Table 1. The densities, viscosities, refractive indices, and surface tensions at T = 298.15 K for the pure components are in good agreement with the accepted literature values (Table 2).[5−18]

Table 1. Chemical Sources, Purities, and Analysis Methods for Pure Components

chemical name	source	initial mass fraction purity	purification method	final mass fraction purity	analysis method
ethanol	Merck	>0.999	molecular sieve	0.999	GC,[a] Karl Fischer[b]
benzyl acetate	Merck	>0.99	molecular sieve	0.997	GC, Karl Fischer
benzyl alcohol	Merck	>0.995	molecular sieve	0.999	GC, Karl Fischer

[a] Gas−liquid chromatography. [b] Karl Fischer moisture meter.

Apparatus and Procedure. The detailed experimental procedure and calibration have been described in our earlier papers,[16,19] so only a brief description of the measurement is presented here. Densities ρ were measured with an Anton Paar DMA-5000 vibrating-tube densimeter (Anton-Paar, Graz, Austria) with an uncertainty of $\pm$ 8·10^{-5} g·cm^{-3}. Viscosities, η, were determined with an automatic microviscometer (Anton Paar type AMVn), which uses the rolling-ball principle. Triplicate measurements of

Received: October 28, 2011
Accepted: February 17, 2012
Published: March 2, 2012

Table 2. Comparison of Measured Densities (ρ), Viscosities (η), Refractive Indices (n_D), and Surface Tensions (σ) of Pure Components with Literature Values at T = 298.15 K[a]

	ρ/g·cm^{-3}		η/mPa·s		n_D		σ/mN·m^{-1}	
component	expt.	lit.	expt.	lit.	expt.	lit.	expt.	lit.
ethanol	0.78507	0.78500[b]	1.090	1.105[b]	1.35934	1.35941[b]	21.9	22.3[b]
		0.78509[c]		1.0826[f]		1.35920[e]		21.8[j]
		0.78515[d]		1.092[g]		1.35922[h]		
		0.78522[e]				1.35950[i]		
benzyl acetate	1.05113	1.05075[b]	2.049	2.056[b]	1.50007	1.49982[b]	36.2	36.4[b]
		1.0515[f]						
benzyl alcohol	1.04134	1.0414[k]	5.376	5.555[m]	1.53848	1.5383[d]	38.5	38.58[k]
		1.04127[f]		5.313[n]		1.53837[f]		38.63[m]
		1.0413[l]				1.53840[l]		38.54[o]
						1.53843[m]		

[a]The standard uncertainties u are $u(T)$ = (0.01, 0.05, 0.03, and 0.05) K for ρ, η, n_D, and σ, respectively, and the combined expanded uncertainties U_c are $U_c(\rho)$ = 0.08 kg·m^{-3}, $U_c(\eta)$ = 0.008 mPa·s, $U_c(n_D)$ = 0.00005, and $U_c(\sigma)$ = 0.2 mN·m^{-1} (level of confidence = 0.95). [b]Sheu and Tu, 2006.[5] [c]Francesconi et al., 1997.[6] [d]Segade et al., 2003.[7] [e]Arce et al., 2000.[8] [f]Riddick et al., 1986.[9] [g]Phillips and Murphy, 1970.[10] [h]Tojo et al., 2001.[11] [i]Chen et al., 2001.[12] [j]Azizian and Bashavard, 2005.[13] [k]Azizian et al., 2006.[14] [l]Singh and Sinha, 1986.[15] [m]Yeh and Tu, 2007.[16] [n]Aralaguppi et al., 2003.[17] [o]Lange, 1985.[18]

flow times were reproducible within ± 0.1 %. The uncertainty of the viscosity measurement was estimated to be better than ± 0.008 mPa·s.

Refractive indices, n_D, were measured with an automatic Anton Paar RXA-156 refractometer, which runs with the wavelength of 589 nm corresponding to the D-ray of sodium with an uncertainty of ± 0.00005. Surface tensions, σ, were measured with an automatic tensionmeter model CBVP-A3 (Kyowa, Japan), which works by the Wilhelmy-plate method. A glass cover with a hole for the thermometer and a short cut for the Wilhelmy-plate was used to cover the vessel for minimizing the errors caused by evaporation losses. The uncertainty of surface tension measurement was estimated at ± 0.2 mN·m^{-1}.

All samples were prepared by mass in a 50 cm^3 Erlenmeyer flask provided with a joint stopper, using a Mettler AB204 balance with a precision of ± 0.1 mg. The possible error of composition in mole fraction was estimated to be ± $1\cdot10^{-4}$. For reducing the time to reach the measuring temperatures, the sample mixtures in airtight stoppered bottles were preheated in a temperature-controlled water bath before being poured into the measuring cell. The bottles were almost completely filled with the liquid mixtures to keep the vapor space above the liquid as small as possible. All liquids were thermostatically controlled under atmospheric pressure (100.8 ± 0.4) kPa to within ± 0.01 K for ρ, ± 0.05 K for η, ± 0.03 K for n_D, and ± 0.05 K for σ.

■ RESULTS AND DISCUSSION

The experimental data of density, ρ, viscosity, η, refractive index, n_D, and surface tension, σ, for the binary systems (ethanol + benzyl acetate, ethanol + benzyl alcohol, and benzyl acetate + benzyl alcohol) at T = (293.15, 303.15, 313.15, and 323.15) K are presented in Tables 3 to 5. Increasing temperatures from (293.15 to 323.15) K decreases the values of ρ, η, n_D, and σ. The experimental ρ, η, n_D, and σ data for the ternary system (ethanol + benzyl acetate + benzyl alcohol) at T = 303.15 K are listed in Table 6. Although the properties (ρ, η, n_D, and σ) of ethanol + benzyl acetate have been measured previously at T = (298.15, 308.15, 318.15, and 328.15) K, the system is repeated mainly because of the designation to have new experimental data at new investigated temperatures to complete this study. The agreement between our present measurements and previous results on this system is generally satisfactory except for viscosity. A fair agreement observed for the viscosity may not be solely due to the present experimental method, which uses the rolling-ball principle instead of the previous Ubbelohde capillary viscometry, since the experimental data may more or less deviate from the true values depending upon the experimental apparatus, procedure, and compounds used.

The experimental ρ, η, n_D, or σ data of pure components at T = (293.15, 303.15, 313.15, and 323.15) K were correlated with temperature by the following equation:

$$Q = B_0 + B_1 T + B_2 T^2 \tag{1}$$

where Q refers to the ρ/g·cm^{-3}, η/mPa·s, n_D, and σ/mN·m^{-1}, and T is the temperature in K. The values of the coefficient B_k together with the standard deviation (δ) are presented in Table 7. The standard deviation is calculated by:

$$\delta = \left[\sum_{i=1}^{n} \frac{(Q_i^{\text{calc}} - Q_i^{\text{expt}})^2}{n - p}\right]^{1/2} \tag{2}$$

where n is the number of data points and p is the number of coefficients used in fitting the data. The standard deviations of ρ, η, n_D, and σ are less than 0.00009 g·cm^{-3}, 0.004 mPa·s, 0.00003, and 0.2 mN·m^{-1}, respectively.

These new experimental data were used to calculate excess molar volumes (V^E), deviations in viscosity ($\Delta\eta$), deviations in refractive index (Δn_D), and deviations in surface tension ($\Delta\sigma$). The molar excess volumes, V^E, were obtained from the experimental density according to the following equation:

$$V^E = \sum_{i=1}^{N} x_i M_i \left(\frac{1}{\rho} - \frac{1}{\rho_i}\right) \tag{3}$$

where x_i, M_i, and ρ_i are the mole fraction, molecular weight, and density of pure component i, respectively. ρ is the density of the mixture, and N is the number of components in the mixture. The uncertainty of V^E was estimated to be within ± $6\cdot10^{-3}$ cm^3·mol^{-1}. The deviations in the viscosity, $\Delta\eta$, were determined from the viscosity of pure component i, η_i, and the viscosity of the mixture, η, as eq 4:

$$\Delta\eta = \eta - \sum_{i=1}^{N} x_i \eta_i \tag{4}$$

dx.doi.org/10.1021/je201009c | J. Chem. Eng. Data 2012, 57, 1118−1127

Table 3. Experimental Densities (ρ), Viscosities (η), Refractive Indices (n_D), Surface Tensions (σ), Excess Molar Volumes (V^E), and Deviations in Viscosities ($\Delta\eta$) for Ethanol (1) + Benzyl Acetate (2) at T = (293.15, 303.15, 313.15, and 323.15) K[a]

x_1	ρ / $g \cdot cm^{-3}$	η / mPa·s	n_D	σ / $mN \cdot m^{-1}$	V^E / $cm^3 \cdot mol^{-1}$	$\Delta\eta$ / mPa·s	x_1	ρ / $g \cdot cm^{-3}$	η / mPa·s	n_D	σ / $mN \cdot m^{-1}$	V^E / $cm^3 \cdot mol^{-1}$	$\Delta\eta$ / mPa·s
						T/K = 293.15							
0.0000	1.05581	2.324	1.50245	37.3	0.000	0.000	0.5499	0.96973	1.439	1.45652	27.9	−0.296	−0.258
0.0502	1.05061	2.180	1.49958	36.3	−0.060	−0.087	0.6000	0.95731	1.392	1.44996	27.2	−0.301	−0.247
0.1000	1.04489	2.063	1.49646	35.4	−0.090	−0.147	0.6500	0.94377	1.347	1.44279	26.7	−0.307	−0.235
0.1498	1.03877	1.962	1.49316	34.4	−0.117	−0.191	0.7000	0.92869	1.305	1.43481	26.2	−0.301	−0.220
0.1998	1.03215	1.879	1.48968	33.4	−0.138	−0.217	0.7499	0.91206	1.267	1.42603	25.8	−0.297	−0.201
0.2499	1.02514	1.808	1.48589	32.5	−0.167	−0.231	0.7999	0.89344	1.232	1.41623	25.2	−0.280	−0.179
0.2998	1.01751	1.736	1.48190	31.6	−0.181	−0.246	0.8500	0.87242	1.202	1.40518	24.5	−0.255	−0.152
0.3500	1.00927	1.672	1.47760	30.8	−0.193	−0.253	0.9000	0.84854	1.188	1.39263	23.8	−0.207	−0.109
0.4000	1.00055	1.613	1.47289	30.0	−0.223	−0.255	0.9500	0.82138	1.178	1.37820	23.1	−0.148	−0.062
0.4501	0.99115	1.551	1.46787	29.3	−0.254	−0.259	1.0000	0.78910	1.183	1.36137	22.3	0.000	0.000
0.5000	0.98094	1.490	1.46245	28.6	−0.281	−0.264							
						T/K = 303.15							
0.0000	1.04674	1.836	1.49776	35.6	0.000	0.000	0.5499	0.95994	1.194	1.45179	27.1	−0.217	−0.171
0.0502	1.04118	1.750	1.49479	34.8	−0.013	−0.043	0.6000	0.94761	1.151	1.44531	26.4	−0.231	−0.171
0.1000	1.03533	1.663	1.49168	34.0	−0.027	−0.087	0.6500	0.93397	1.115	1.43815	25.8	−0.227	−0.165
0.1498	1.02909	1.595	1.48838	33.2	−0.040	−0.113	0.7000	0.91903	1.077	1.43018	25.2	−0.233	−0.160
0.1998	1.02242	1.534	1.48491	32.4	−0.056	−0.131	0.7499	0.90250	1.038	1.42142	24.7	−0.235	−0.156
0.2499	1.01530	1.477	1.48118	31.6	−0.074	−0.145	0.7999	0.88390	1.009	1.41163	24.2	−0.218	−0.142
0.2998	1.00778	1.420	1.47715	30.8	−0.103	−0.159	0.8500	0.86307	0.989	1.40062	23.6	−0.204	−0.119
0.3500	0.99968	1.375	1.47284	30.0	−0.132	−0.161	0.9000	0.83936	0.982	1.38811	22.9	−0.163	−0.084
0.4000	0.99086	1.327	1.46818	29.2	−0.150	−0.167	0.9500	0.81221	0.975	1.37384	22.2	−0.098	−0.048
0.4501	0.98138	1.281	1.46316	28.5	−0.175	−0.170	1.0000	0.78076	0.980	1.35712	21.4	0.000	0.000
0.5000	0.97111	1.233	1.45772	27.8	−0.196	−0.175							
						T/K = 313.15							
0.0000	1.03742	1.474	1.49309	34.3	0.000	0.000	0.5499	0.95019	0.999	1.44703	26.4	−0.173	−0.116
0.0502	1.03185	1.413	1.49006	33.6	−0.012	−0.028	0.6000	0.93783	0.964	1.44052	25.8	−0.184	−0.119
0.1000	1.02596	1.362	1.48693	32.8	−0.022	−0.047	0.6500	0.92436	0.930	1.43339	25.2	−0.196	−0.120
0.1498	1.01970	1.308	1.48362	32.0	−0.033	−0.068	0.7000	0.90951	0.891	1.42552	24.6	−0.208	−0.127
0.1998	1.01298	1.265	1.48007	31.3	−0.042	−0.079	0.7499	0.89304	0.867	1.41682	24.0	−0.214	−0.118
0.2499	1.00582	1.226	1.47629	30.5	−0.057	−0.085	0.7999	0.87460	0.841	1.40711	23.4	−0.207	−0.111
0.2998	0.99820	1.181	1.47228	29.8	−0.072	−0.098	0.8500	0.85375	0.823	1.39617	22.8	−0.186	−0.097
0.3500	0.98997	1.143	1.46794	29.1	−0.089	−0.103	0.9000	0.83017	0.812	1.38375	22.1	−0.151	−0.075
0.4000	0.98120	1.101	1.46327	28.4	−0.114	−0.112	0.9500	0.80327	0.808	1.36951	21.4	−0.097	−0.047
0.4501	0.97170	1.067	1.45826	27.7	−0.137	−0.114	1.0000	0.77199	0.822	1.35292	20.6	0.000	0.000
0.5000	0.96142	1.029	1.45286	27.0	−0.158	−0.119							
						T/K = 323.15							
0.0000	1.02751	1.256	1.48834	33.2	0.000	0.000	0.5499	0.94031	0.882	1.44215	25.3	−0.159	−0.067
0.0502	1.02188	1.220	1.48521	32.5	−0.002	−0.008	0.6000	0.92798	0.853	1.43561	24.7	−0.169	−0.068
0.1000	1.01597	1.187	1.48205	31.8	−0.009	−0.013	0.6500	0.91458	0.825	1.42851	24.1	−0.185	−0.068
0.1498	1.00969	1.154	1.47874	31.1	−0.016	−0.018	0.7000	0.89972	0.795	1.42067	23.5	−0.193	−0.070
0.1998	1.00294	1.120	1.47517	30.4	−0.020	−0.025	0.7499	0.88326	0.770	1.41198	22.9	−0.194	−0.068
0.2499	0.99585	1.086	1.47143	29.6	−0.043	−0.031	0.7999	0.86486	0.743	1.40231	22.3	−0.185	−0.067
0.2998	0.98826	1.050	1.46739	28.9	−0.062	−0.039	0.8500	0.84415	0.723	1.39132	21.7	−0.170	−0.059
0.3500	0.98003	1.015	1.46309	28.2	−0.076	−0.046	0.9000	0.82071	0.704	1.37895	21.0	−0.137	−0.050
0.4000	0.97124	0.979	1.45847	27.5	−0.097	−0.054	0.9500	0.79402	0.692	1.36489	20.3	−0.088	−0.034
0.4501	0.96172	0.943	1.45346	26.7	−0.116	−0.062	1.0000	0.76303	0.698	1.34873	19.4	0.000	0.000
0.5000	0.95149	0.911	1.44807	26.0	−0.141	−0.066							

[a]The standard uncertainties u are $u(T)$ = (0.01, 0.05, 0.03, and 0.05) K for ρ, η, n_D, and σ, respectively, and the combined expanded uncertainties U_c are $U_c(\rho) = 0.08\ kg \cdot m^{-3}$, $U_c(\eta) = 0.008$ mPa·s, $U_c(n_D) = 0.00005$, $U_c(\sigma) = 0.2\ mN \cdot m^{-1}$, and $U_c(V^E) = 0.006\ cm^3 \cdot mol^{-1}$ (level of confidence = 0.95).

The deviation in the refractive index, Δn_D, was calculated on a volume fraction basis in which case it has simple theoretical significance as reflecting changes in free volume, as stated by Brocos et al.,[20] and is given by:

$$\Delta n_D = n_D - \sum_{i=1}^{N} \phi_i n_{Di} \tag{5}$$

where n_D is the refractive index of the mixture. n_{Di} and ϕ_i are the refractive index and the volume fraction of pure component i, respectively. The volume fraction, ϕ_i, is defined by:

$$\phi_i = \frac{x_i(M_i/\rho_i)}{\sum_{j=1}^{N} x_j(M_j/\rho_j)} \tag{6}$$

Table 4. Experimental Densities (ρ), Viscosities (η), Refractive Indices (n_D), Surface Tensions (σ), Excess Molar Volumes (V^E), and Deviations in Viscosity ($\Delta\eta$) for Ethanol (1) + Benzyl Alcohol (3) at T = (293.15, 303.15, 313.15, and 323.15) K[a]

x_1	ρ g·cm^{-3}	η mPa·s	n_D	σ mN·m^{-1}	V^E cm^3·mol^{-1}	$\Delta\eta$ mPa·s	x_1	ρ g·cm^{-3}	η mPa·s	n_D	σ mN·m^{-1}	V^E cm^3·mol^{-1}	$\Delta\eta$ mPa·s
						T/K = 293.15							
0.0000	1.04544	6.287	1.54049	39.2	0.000	0.000	0.5500	0.94823	2.857	1.47074	30.9	−0.617	−0.623
0.0500	1.03893	5.903	1.53607	38.7	−0.086	−0.129	0.5999	0.93557	2.623	1.46176	29.9	−0.623	−0.602
0.1000	1.03201	5.548	1.53119	38.1	−0.162	−0.229	0.6500	0.92193	2.392	1.45220	28.9	−0.617	−0.577
0.1504	1.02472	5.197	1.52584	37.5	−0.242	−0.322	0.6997	0.90734	2.169	1.44199	28.0	−0.596	−0.547
0.1999	1.01709	4.871	1.52041	36.8	−0.309	−0.396	0.7500	0.89149	1.971	1.43095	27.1	−0.563	−0.488
0.2502	1.00895	4.550	1.51444	36.1	−0.377	−0.460	0.7999	0.87442	1.782	1.41922	26.1	−0.509	−0.422
0.3003	1.00031	4.236	1.50804	35.3	−0.435	−0.518	0.8496	0.85594	1.611	1.40661	25.2	−0.435	−0.340
0.3499	0.99124	3.940	1.50154	34.5	−0.489	−0.561	0.8998	0.83544	1.454	1.39275	24.3	−0.307	−0.240
0.3998	0.98152	3.655	1.49454	33.6	−0.533	−0.591	0.9500	0.81326	1.305	1.37776	23.3	−0.171	−0.133
0.4500	0.97112	3.377	1.48707	32.7	−0.570	−0.613	1.0000	0.78910	1.183	1.36137	22.3	0.000	0.000
0.5001	0.96001	3.107	1.47910	31.8	−0.597	−0.627							
						T/K = 303.15							
0.0000	1.03745	4.579	1.53635	38.1	0.000	0.000	0.5500	0.93995	2.206	1.46632	29.8	−0.629	−0.394
0.0500	1.03091	4.276	1.53175	37.5	−0.087	−0.123	0.5999	0.92733	2.030	1.45731	28.8	−0.624	−0.390
0.1000	1.02402	4.006	1.52681	36.9	−0.168	−0.213	0.6500	0.91364	1.873	1.44770	27.8	−0.621	−0.367
0.1504	1.01676	3.761	1.52150	36.2	−0.248	−0.277	0.6997	0.89899	1.716	1.43754	26.9	−0.598	−0.345
0.1999	1.00906	3.529	1.51591	35.5	−0.311	−0.331	0.7500	0.88314	1.568	1.42651	26.0	−0.567	−0.312
0.2502	1.00090	3.321	1.51002	34.8	−0.390	−0.358	0.7999	0.86599	1.423	1.41479	25.1	−0.508	−0.277
0.3003	0.99229	3.117	1.50367	34.1	−0.447	−0.381	0.8496	0.84751	1.292	1.40202	24.2	−0.437	−0.229
0.3499	0.98316	2.924	1.49716	33.3	−0.496	−0.396	0.8998	0.82713	1.173	1.38825	23.3	−0.312	−0.168
0.3998	0.97334	2.735	1.49014	32.5	−0.548	−0.405	0.9500	0.80504	1.060	1.37331	22.3	−0.183	−0.100
0.4500	0.96291	2.542	1.48260	31.6	−0.599	−0.414	1.0000	0.78076	0.980	1.35712	21.4	0.000	0.000
0.5001	0.95176	2.368	1.47469	30.7	−0.607	−0.411							
						T/K = 313.15							
0.0000	1.02961	3.335	1.53215	37.2	0.000	0.000	0.5500	0.93178	1.684	1.46191	28.9	−0.638	−0.269
0.0500	1.02304	3.171	1.52743	36.6	−0.089	−0.038	0.5999	0.91904	1.561	1.45296	27.9	−0.642	−0.266
0.1000	1.01621	3.002	1.52250	35.9	−0.170	−0.082	0.6500	0.90541	1.441	1.44333	26.9	−0.637	−0.261
0.1504	1.00886	2.841	1.51718	35.3	−0.256	−0.116	0.6997	0.89069	1.332	1.43309	26.0	−0.608	−0.245
0.1999	1.00116	2.688	1.51156	34.6	−0.328	−0.145	0.7500	0.87475	1.236	1.42212	25.1	−0.583	−0.214
0.2502	0.99296	2.539	1.50560	33.9	−0.392	−0.167	0.7999	0.85751	1.146	1.41040	24.2	−0.523	−0.179
0.3003	0.98428	2.389	1.49935	33.2	−0.470	−0.191	0.8496	0.83883	1.048	1.39761	23.3	−0.430	−0.152
0.3499	0.97505	2.244	1.49265	32.4	−0.496	−0.212	0.8998	0.81848	0.972	1.38389	22.4	−0.326	−0.102
0.3998	0.96524	2.101	1.48568	31.6	−0.551	−0.229	0.9500	0.79632	0.899	1.36905	21.5	−0.219	−0.049
0.4500	0.95484	1.955	1.47818	30.7	−0.591	−0.249	1.0000	0.77199	0.822	1.35292	20.6	0.000	0.000
0.5001	0.94367	1.819	1.47030	29.8	−0.618	−0.259							
						T/K = 323.15							
0.0000	1.02150	2.545	1.52796	36.3	0.000	0.000	0.5500	0.92328	1.462	1.45755	27.8	−0.698	−0.067
0.0500	1.01486	2.439	1.52308	35.6	−0.091	−0.014	0.5999	0.91048	1.368	1.44855	26.8	−0.695	−0.069
0.1000	1.00798	2.337	1.51807	34.9	−0.189	−0.023	0.6500	0.89661	1.279	1.43892	25.8	−0.685	−0.065
0.1504	1.00057	2.238	1.51273	34.2	−0.275	−0.029	0.6997	0.88189	1.189	1.42870	24.8	−0.658	−0.064
0.1999	0.99289	2.142	1.50721	33.5	−0.353	−0.034	0.7500	0.86588	1.105	1.41775	23.9	−0.622	−0.055
0.2502	0.98467	2.041	1.50123	32.8	−0.431	−0.042	0.7999	0.84864	1.022	1.40607	23.0	−0.557	−0.046
0.3003	0.97599	1.941	1.49494	32.1	−0.515	−0.049	0.8496	0.83007	0.937	1.39329	22.1	−0.461	−0.039
0.3499	0.96671	1.844	1.48825	31.3	−0.541	−0.055	0.8998	0.80962	0.854	1.37963	21.2	−0.350	−0.029
0.3998	0.95684	1.746	1.48127	30.5	−0.598	−0.061	0.9500	0.78741	0.774	1.36475	20.3	−0.232	−0.016
0.4500	0.94637	1.649	1.47378	29.6	−0.636	−0.065	1.0000	0.76303	0.698	1.34873	19.4	0.000	0.000
0.5001	0.93523	1.556	1.46589	28.7	−0.682	−0.065							

[a] The standard uncertainties u are $u(T)$ = (0.01, 0.05, 0.03, and 0.05) K for ρ, η, n_D, and σ, respectively, and the combined expanded uncertainties U_c are $U_c(\rho)$ = 0.08 kg·m^{-3}, $U_c(\eta)$ = 0.008 mPa·s, $U_c(n_D)$ = 0.00005, $U_c(\sigma)$ = 0.2 mN·m^{-1}, and $U_c(V^E)$ = 0.006 cm^3·mol^{-1} (level of confidence = 0.95).

where x_i, M_i, and ρ_i are the mole fraction, molecular weight, and density of pure component i, respectively. The deviations in surface tension, $\Delta\sigma$, were evaluated from the following equation:

$$\Delta\sigma = \sigma - \sum_{i=1}^{N} x_i\sigma_i \tag{7}$$

where σ and σ_i are the surface tensions of the mixture and pure liquid i, respectively.

All of the binary quantities (V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$) have been fitted to the Redlich−Kister equation[21] by the method of least-squares, to derive the binary coefficients (a_k) and standard deviation (δ):

$$\Delta Q_{ij} = x_i x_j \sum_{k=0}^{m} a_k (x_i - x_j)^k \tag{8}$$

Table 5. Experimental Densities (ρ), Viscosities (η), Refractive Indices (n_D), Surface Tensions (σ), Excess Molar Volumes (V^E), and Deviations in Viscosity ($\Delta\eta$) for Benzyl Acetate (2) + Benzyl Alcohol (3) at T = (293.15, 303.15, 313.15, and 323.15) K[a]

x_2	ρ / g·cm^{-3}	η / mPa·s	n_D	σ / mN·m^{-1}	V^E / cm^3·mol^{-1}	$\Delta\eta$ / mPa·s	x_2	ρ / g·cm^{-3}	η / mPa·s	n_D	σ / mN·m^{-1}	V^E / cm^3·mol^{-1}	$\Delta\eta$ / mPa·s
						T/K = 293.15							
0.0000	1.04544	6.287	1.54049	39.2	0.000	0.000	0.5501	1.05226	2.930	1.51710		−0.038	−1.177
0.0500	1.04629	5.782	1.53821		−0.015	−0.307	0.6001	1.05274	2.795	1.51530	38.4	−0.038	−1.114
0.1001	1.04703	5.319	1.53584	39.2	−0.022	−0.571	0.6500	1.05319	2.684	1.51352		−0.037	−1.027
0.1502	1.04773	4.905	1.53352		−0.028	−0.787	0.6999	1.05364	2.589	1.51182	38.1	−0.036	−0.924
0.2001	1.04838	4.536	1.53127	39.2	−0.030	−0.958	0.7502	1.05403	2.505	1.51014		−0.031	−0.809
0.2500	1.04899	4.214	1.52907		−0.031	−1.082	0.8000	1.05442	2.428	1.50852	37.8	−0.027	−0.689
0.3000	1.04958	3.927	1.52689	39.1	−0.032	−1.171	0.8500	1.05477	2.376	1.50696		−0.019	−0.542
0.3498	1.05015	3.678	1.52480		−0.033	−1.223	0.9000	1.05511	2.343	1.50544	37.5	−0.010	−0.377
0.4001	1.05071	3.454	1.52279	39.0	−0.035	−1.247	0.9500	1.05546	2.326	1.50396		−0.004	−0.196
0.4500	1.05124	3.252	1.52083		−0.036	−1.252	1.0000	1.05581	2.324	1.50245	37.3	0.000	0.000
0.5000	1.05177	3.087	1.51893	38.7	−0.038	−1.219							
						T/K = 303.15							
0.0000	1.03745	4.579	1.53635	38.1	0.000	0.000	0.5501	1.04343	2.332	1.51239		−0.019	−0.738
0.0500	1.03818	4.210	1.53390		−0.010	−0.232	0.6001	1.04384	2.234	1.51057	36.7	−0.016	−0.699
0.1001	1.03883	3.894	1.53143	38.0	−0.015	−0.410	0.6500	1.04424	2.171	1.50881		−0.014	−0.625
0.1502	1.03944	3.623	1.52903		−0.018	−0.544	0.6999	1.04462	2.091	1.50711	36.3	−0.011	−0.568
0.2001	1.04001	3.378	1.52673	37.9	−0.020	−0.652	0.7502	1.04499	2.035	1.50545		−0.008	−0.486
0.2500	1.04058	3.165	1.52449		−0.023	−0.728	0.8000	1.04535	1.985	1.50383	36.0	−0.005	−0.400
0.3000	1.04111	2.972	1.52231	37.8	−0.024	−0.784	0.8500	1.04570	1.941	1.50227		−0.002	−0.306
0.3498	1.04161	2.806	1.52022		−0.024	−0.813	0.9000	1.04605	1.902	1.50075	35.8	−0.001	−0.208
0.4001	1.04210	2.662	1.51819	37.5	−0.024	−0.820	0.9500	1.04640	1.867	1.49926		−0.001	−0.106
0.4500	1.04257	2.535	1.51621		−0.023	−0.810	1.0000	1.04674	1.836	1.49776	35.6	0.000	0.000
0.5000	1.04301	2.432	1.51428	37.1	−0.021	−0.776							
						T/K = 313.15							
0.0000	1.02961	3.335	1.53215	37.2	0.000	0.000	0.5501	1.03460	1.903	1.50774		−0.008	−0.419
0.0500	1.03021	3.180	1.52962		−0.008	−0.062	0.6001	1.03494	1.832	1.50590	35.2	−0.006	−0.386
0.1001	1.03076	3.006	1.52715	37.0	−0.011	−0.143	0.6500	1.03527	1.774	1.50410		−0.003	−0.351
0.1502	1.03127	2.848	1.52471		−0.014	−0.207	0.6999	1.03557	1.728	1.50237	34.8	0.002	−0.304
0.2001	1.03172	2.687	1.52235	36.8	−0.016	−0.276	0.7502	1.03587	1.684	1.50070		0.006	−0.255
0.2500	1.03223	2.536	1.52007		−0.018	−0.334	0.8000	1.03618	1.646	1.49906	34.6	0.007	−0.200
0.3000	1.03267	2.396	1.51785	36.4	−0.018	−0.381	0.8500	1.03648	1.613	1.49748		0.008	−0.140
0.3498	1.03308	2.265	1.51571		−0.017	−0.419	0.9000	1.03679	1.572	1.49596	34.4	0.007	−0.088
0.4001	1.03348	2.154	1.51362	36.0	−0.015	−0.436	0.9500	1.03711	1.524	1.49450		0.004	−0.043
0.4500	1.03386	2.056	1.51160		−0.013	−0.442	1.0000	1.03742	1.474	1.49309	34.3	0.000	0.000
0.5000	1.03424	1.966	1.50964	35.6	−0.012	−0.439							
						T/K = 323.15							
0.0000	1.02150	2.545	1.52796	36.3	0.000	0.000	0.5501	1.02528	1.561	1.50314		−0.001	−0.275
0.0500	1.02194	2.450	1.52532		−0.004	−0.031	0.6001	1.02553	1.521	1.50128	33.9	0.003	−0.250
0.1001	1.02236	2.349	1.52278	36.0	−0.007	−0.067	0.6500	1.02579	1.482	1.49946		0.005	−0.225
0.1502	1.02275	2.232	1.52030		−0.008	−0.119	0.6999	1.02604	1.444	1.49771	33.5	0.007	−0.199
0.2001	1.02312	2.125	1.51791	35.7	−0.009	−0.162	0.7502	1.02628	1.410	1.49598		0.008	−0.168
0.2500	1.02348	2.021	1.51560		−0.009	−0.202	0.8000	1.02652	1.387	1.49434	33.4	0.009	−0.127
0.3000	1.02381	1.925	1.51335	35.2	−0.009	−0.233	0.8500	1.02677	1.361	1.49276		0.009	−0.088
0.3498	1.02413	1.838	1.51118		−0.008	−0.256	0.9000	1.02701	1.339	1.49124	33.3	0.008	−0.046
0.4001	1.02444	1.756	1.50908	34.8	−0.007	−0.273	0.9500	1.02726	1.308	1.48976		0.004	−0.012
0.4500	1.02473	1.683	1.50704		−0.005	−0.282	1.0000	1.02751	1.256	1.48834	33.2	0.000	0.000
0.5000	1.02502	1.620	1.50506	34.3	−0.004	−0.281							

[a] The standard uncertainties u are $u(T)$ = (0.01, 0.05, 0.03, and 0.05) K for ρ, η, n_D, and σ, respectively, and the combined expanded uncertainties U_c are $U_c(\rho)$ = 0.08 kg·m^{-3}, $U_c(\eta)$ = 0.008 mPa·s, $U_c(n_D)$ = 0.00005, $U_c(\sigma)$ = 0.2 mN·m^{-1}, and $U_c(V^E)$ = 0.006 cm^3·mol^{-1} (level of confidence = 0.95).

where ΔQ_{ij} refers to the binary V^E/cm^3·mol^{-1}, $\Delta\eta$/mPa·s, Δn_D, or $\Delta\sigma$/mN·m^{-1} for the $i + j$ system and $x_j = 1 - x_i$. In each case, the optimum number of coefficients (a_k) was determined from an examination of the residuals as a function of composition and the variation of standard deviation (δ) as defined in eq 2. Estimated values of a_k and δ for V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$ are presented in Table 8. For the case of V^E, the δ values lie between $5 \cdot 10^{-4}$ cm^3·mol^{-1} and $6 \cdot 10^{-3}$ cm^3·mol^{-1}, and the largest δ value corresponds to ethanol + benzyl acetate at T = 293.15 K.

The derived data, V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$, for the ternary system of ethanol (1) + benzyl acetate (2) + benzyl alcohol (3) at T = 303.15 K were correlated respectively using the equation:

$$\Delta Q_{123} = \Delta Q_{12} + \Delta Q_{13} + \Delta Q_{23} + x_1 x_2 x_3 \Delta_{123} \qquad (9)$$

dx.doi.org/10.1021/je201009c | J. Chem. Eng. Data 2012, 57, 1118−1127

Table 6. Experimental Densities (ρ), Viscosities (η), Refractive Indices (n_D), Surface Tensions (σ), Excess Molar Volumes (V^E), and Deviations in Viscosity ($\Delta\eta$) for Ethanol (1) + Benzyl Acetate (2) + Benzyl Alcohol (3) at T = 303.15 K[a]

x_1	x_2	ρ (g·cm^{-3})	η (mPa·s)	n_D	σ (mN·m^{-1})	V^E (cm^3·mol^{-1})	$\Delta\eta$ (mPa·s)	x_1	x_2	ρ (g·cm^{-3})	η (mPa·s)	n_D	σ (mN·m^{-1})	V^E (cm^3·mol^{-1})	$\Delta\eta$ (mPa·s)
0.0494	0.9006	1.04085	1.774	1.49634	35.0	−0.015	−0.157	0.3011	0.5491	1.00517	1.576	1.48187	31.5	−0.207	−0.413
0.0498	0.8002	1.04002	1.854	1.49939	35.2	−0.029	−0.351	0.3000	0.4499	1.00350	1.714	1.48542	31.9	−0.266	−0.551
0.0496	0.7001	1.03920	1.954	1.50265	35.5	−0.043	−0.526	0.3008	0.3496	1.00139	1.896	1.48895	32.5	−0.327	−0.641
0.0502	0.6000	1.03828	2.090	1.50605	35.9	−0.062	−0.663	0.3001	0.2502	0.99925	2.125	1.49290	33.1	−0.373	−0.688
0.0502	0.5002	1.03732	2.258	1.50972	36.3	−0.075	−0.768	0.2996	0.1503	0.99674	2.450	1.49705	33.6	−0.407	−0.638
0.0499	0.4000	1.03631	2.495	1.51362	36.7	−0.085	−0.807	0.3006	0.0200	0.99275	2.999	1.50268	34.1	−0.433	−0.443
0.0502	0.2998	1.03512	2.773	1.51772	37.0	−0.092	−0.803	0.3999	0.5499	0.98984	1.373	1.46975	29.5	−0.187	−0.258
0.0496	0.2000	1.03394	3.145	1.52216	37.3	−0.096	−0.707	0.4011	0.4491	0.98737	1.487	1.47296	30.0	−0.285	−0.417
0.0506	0.1000	1.03239	3.631	1.52673	37.4	−0.094	−0.492	0.3999	0.3501	0.98496	1.655	1.47647	30.6	−0.352	−0.524
0.0504	0.0499	1.03165	3.929	1.52919	37.5	−0.091	−0.332	0.3996	0.2504	0.98222	1.849	1.48013	31.2	−0.425	−0.605
0.1003	0.8494	1.03479	1.701	1.49310	34.2	−0.032	−0.187	0.4000	0.1500	0.97886	2.129	1.48386	31.8	−0.477	−0.599
0.1010	0.7488	1.03382	1.779	1.49623	34.4	−0.061	−0.383	0.4005	0.0498	0.97508	2.499	1.48787	32.3	−0.519	−0.502
0.1005	0.6497	1.03293	1.888	1.49961	34.8	−0.088	−0.547	0.5001	0.4497	0.96956	1.297	1.45928	28.1	−0.241	−0.249
0.1010	0.5495	1.03181	2.027	1.50308	35.2	−0.110	−0.681	0.4997	0.3502	0.96652	1.428	1.46247	28.6	−0.349	−0.392
0.1004	0.4498	1.03076	2.215	1.50687	35.6	−0.132	−0.769	0.5001	0.2500	0.96292	1.602	1.46574	29.3	−0.444	−0.491
0.1011	0.3494	1.02944	2.461	1.51075	36.1	−0.153	−0.796	0.4999	0.1501	0.95893	1.836	1.46913	29.9	−0.522	−0.532
0.1010	0.2500	1.02809	2.751	1.51495	36.4	−0.167	−0.779	0.4996	0.0502	0.95430	2.166	1.47281	30.5	−0.574	−0.477
0.1008	0.1497	1.02653	3.170	1.51945	36.6	−0.170	−0.636	0.6000	0.3501	0.94548	1.214	1.44675	26.8	−0.283	−0.245
0.1008	0.0499	1.02479	3.690	1.52419	36.8	−0.169	−0.389	0.6003	0.2498	0.94105	1.360	1.44960	27.4	−0.408	−0.373
0.2007	0.7492	1.02172	1.569	1.48637	32.6	−0.080	−0.233	0.6001	0.1499	0.93603	1.565	1.45262	28.0	−0.507	−0.443
0.2007	0.6491	1.02055	1.662	1.48961	32.9	−0.133	−0.414	0.6000	0.0501	0.93033	1.848	1.45572	28.6	−0.588	−0.434
0.2002	0.5499	1.01932	1.794	1.49307	33.3	−0.179	−0.556	0.6999	0.2500	0.91623	1.144	1.43151	25.6	−0.306	−0.230
0.2010	0.4496	1.01774	1.952	1.49664	33.8	−0.218	−0.670	0.7002	0.1498	0.90994	1.310	1.43386	26.2	−0.443	−0.338
0.2003	0.3500	1.01621	2.161	1.50049	34.3	−0.250	−0.737	0.7002	0.0500	0.90276	1.556	1.43633	26.7	−0.545	−0.366
0.2006	0.2497	1.01446	2.429	1.50447	34.8	−0.288	−0.743	0.8000	0.1499	0.87984	1.081	1.41253	24.5	−0.298	−0.208
0.2007	0.1496	1.01235	2.786	1.50885	35.2	−0.301	−0.660	0.8000	0.0501	0.87095	1.284	1.41408	25.0	−0.436	−0.278
0.2001	0.0497	1.01017	3.254	1.51350	35.5	−0.312	−0.469	0.9000	0.0500	0.83350	1.056	1.38825	23.2	−0.250	−0.147
0.3006	0.6492	1.00685	1.461	1.47869	31.1	−0.134	−0.255								

[a]The standard uncertainties u are $u(T)$ = (0.01, 0.05, 0.03, and 0.05) K for ρ, η, n_D, and σ, respectively, and the combined expanded uncertainties U_c are $U_c(\rho)$ = 0.08 kg·m^{-3}, $U_c(\eta)$ = 0.008 mPa·s, $U_c(n_D)$ = 0.00005, $U_c(\sigma)$ = 0.2 mN·m^{-1}, and $U_c(V^E)$ = 0.006 cm^3·mol^{-1} (level of confidence = 0.95).

Table 7. Coefficients (B_k) and Standard Deviations (δ) of Equation 1 in the Correlation of ρ, η, n_D, and σ for the Pure Components from T = (293.15 to 323.15) K

component	Q	B_0	$B_1 \cdot 10^3$	$B_2 \cdot 10^6$	$\delta \cdot 10^3$
ethanol	ρ/g·cm^{-3}	0.897	0.085	−1.550	0.05
	η/mPa·s	24.620	−137.849	197.500	2.5
	n_D	1.499	−0.514	0.150	0.009
	σ/mN·m^{-1}	−20.924	367.225	−750.000	112
benzyl acetate	ρ/g·cm^{-3}	1.133	0.352	−2.100	0.07
	η/mPa·s	76.722	−451.663	675.000	4.0
	n_D	1.626	−0.377	−0.150	0.02
	σ/mN·m^{-1}	219.255	−1060.450	1500.000	45
benzyl alcohol	ρ/g·cm^{-3}	1.250	−0.612	−0.300	0.09
	η/mPa·s	260.251	−1539.110	2295.000	2.2
	n_D	1.651	−0.341	−0.125	0.02
	σ/mN·m^{-1}	114.698	−404.150	500.000	45

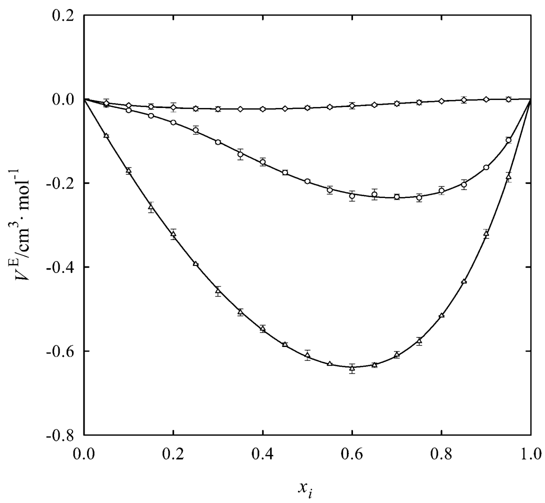


Figure 1. Variation of V^E with x_i at T = 303.15 K: ○, ethanol (1) + benzyl acetate (2), $x_i = x_1$; △, ethanol (1) + benzyl alcohol (3), $x_i = x_1$; ◇, benzyl acetate (2) + benzyl alcohol (3), $x_i = x_2$; solid lines calculated from the Redlich–Kister equation.

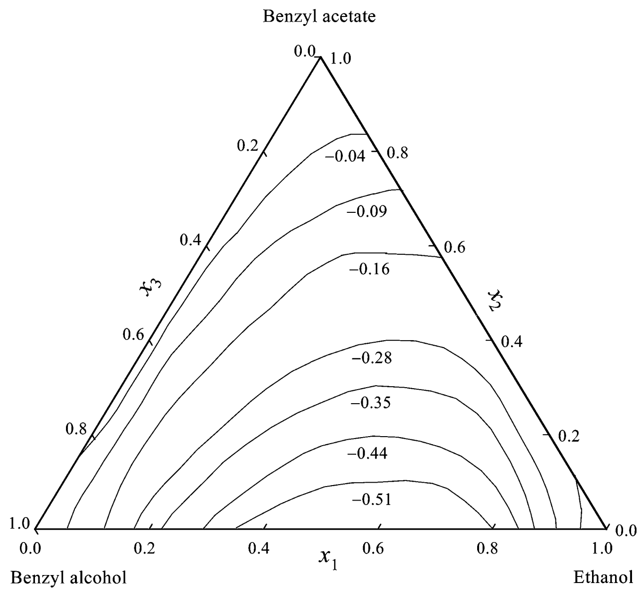


Figure 3. Curves of constant V^E/cm^3·mol^{-1} for the ternary system of ethanol (1) + benzyl acetate (2) + benzyl alcohol (3) at T = 303.15 K.

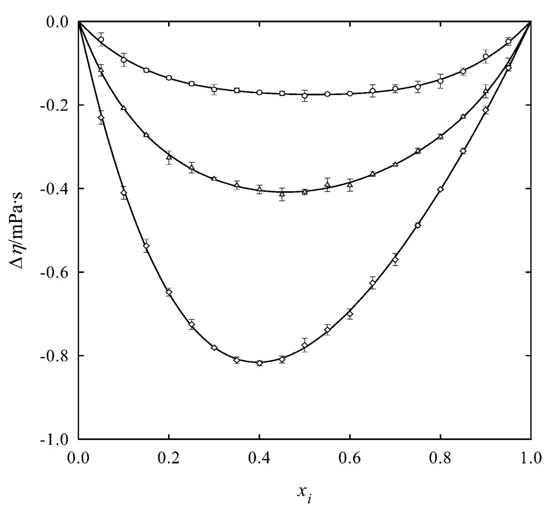


Figure 2. Variation of $\Delta\eta$ with x_i at T = 303.15 K: ○, ethanol (1) + benzyl acetate (2), $x_i = x_1$; △, ethanol (1) + benzyl alcohol (3), $x_i = x_1$; ◇, benzyl acetate (2) + benzyl alcohol (3), $x_i = x_2$; solid lines calculated from the Redlich–Kister equation.

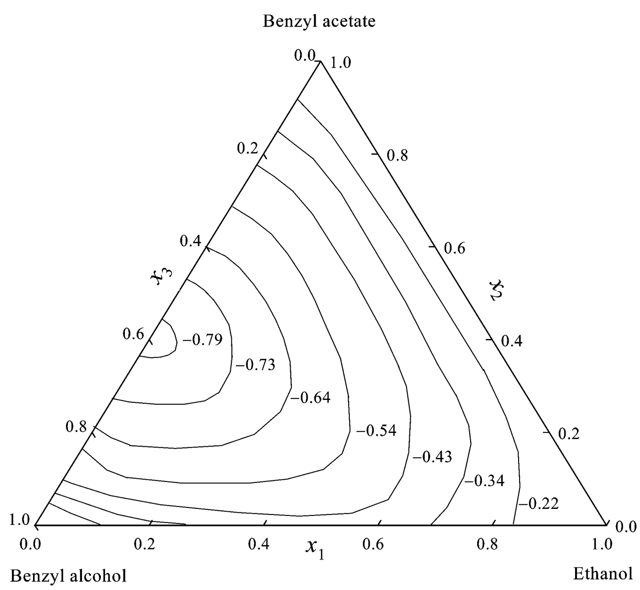


Figure 4. Curves of constant $\Delta\eta$/mPa·s for the ternary system of ethanol (1) + benzyl acetate (2) + benzyl alcohol (3) at T = 303.15 K.

Table 8. Coefficients (a_k) of the Redlich–Kister Equation for the Binary Systems at T = (293.15, 303.15, 313.15, and 323.15) K and Coefficients (C_k) of the Cilbulka Equation for the Ternary System at T = 303.15 K in the Correlation of V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$

ΔQ_{ij}	T/K	a_0	a_1	a_2	a_3	a_4	$\delta\cdot 10^3$
			Ethanol (1) + Benzyl Acetate (2)				
V^E/cm^3·mol^{-1}	293.15	−1.1028	−0.7142	−0.0560	−0.1554	−1.4039	5.7
	303.15	−0.7894	−0.7418	0.0281	−0.3271	−0.6755	3.2
	313.15	−0.6168	−0.7629	−0.2530	−0.2347	−0.4860	2.6
	323.15	−0.5556	−0.7562	−0.1808	−0.2384	−0.3413	2.7
$\Delta\eta$/mPa·s	293.15	−1.0272	0.1015	−0.5956	0.2497		3.6
	303.15	−0.6886	−0.0334	−0.4285			2.9
	313.15	−0.4655	−0.1633	−0.3552			3.1
	323.15	−0.2489	−0.1484	−0.1191	−0.1796		2.8
Δn_D	293.15	0.0042	0.0045	0.0013	0.0039	0.0064	0.03
	303.15	0.0038	0.0044	0.0016	0.0041	0.0039	0.03
	313.15	0.0028	0.0051	0.0021	0.0040	0.0045	0.03
	323.15	0.0020	0.0044	0.0010	0.0019		0.02
$\Delta\sigma$/mN·m^{-1}	293.15	−4.9557	3.5392	4.6139			59
	303.15	−2.9350	0.5057	4.2544	2.5480		40
	313.15	−1.6428	1.7773	2.6885			25
	323.15	−1.1115	0.0872	3.7961	2.7768		27
			Ethanol (1) + Benzyl Alcohol (3)				
V^E/cm^3·mol^{-1}	293.15	−2.3929	−0.9472	−0.4272	−0.1506		3.3
	303.15	−2.4559	−0.9090	−0.4907	−0.2215		3.4
	313.15	−2.5904	−1.0231	−0.4989			4.2
	323.15	−2.6916	−0.9555	−0.4520	−0.2944		4.1
$\Delta\eta$/mPa·s	293.15	−2.4895	−0.1254	−0.2017			3.9
	303.15	−1.6201	0.2073	−0.7518	0.1423		4.2
	313.15	−1.0404	−0.3618	−0.0489	0.3637		3.7
	323.15	−0.2683	−0.0860	0.0756	0.0709	−0.1501	1.3
Δn_D	293.15	0.0131	0.0040	0.0045	0.0006	0.0037	0.03
	303.15	0.0126	0.0043	0.0041			0.04
	313.15	0.0123	0.0051	0.0032	−0.0012		0.04
	323.15	0.0121	0.0054	0.0022			0.05
$\Delta\sigma$/mN·m^{-1}	293.15	4.1560	−3.5948	1.1099	2.1027		27
	303.15	3.7980	−3.3624	−1.8601	2.8776	2.4732	38
	313.15	3.6069	−3.7142	−2.0578	3.2503	1.6655	29
	323.15	3.4408	−3.3592	−3.7809	3.4379	2.9706	25
			Benzyl Acetate (2) + Benzyl Alcohol (3)				
V^E/cm^3·mol^{-1}	293.15	−0.1500	−0.0530	−0.0636	0.2103		0.7
	303.15	−0.0856	0.0711	0.0395	0.0362	−0.0718	0.5
	313.15	−0.0500	0.1044	0.0444			0.7
	323.15	−0.0110	0.0953	0.0296			0.5
$\Delta\eta$/mPa·s	293.15	−4.8936	1.4784	−0.6168	−0.2073		3.7
	303.15	−3.1271	1.2788	−0.4623	0.1493		4.6
	313.15	−1.7515	0.5035	0.7552	−0.2670		2.7
	323.15	−1.1300	0.1875	0.6863			4.5
Δn_D	293.15	0.0019	−0.0008	0.0001	−0.0016	0.0028	0.01
	303.15	0.0011	−0.0006	−0.0005	−0.0000	0.0023	0.01
	313.15	0.0005	−0.0010	0.0000	−0.0009	0.0005	0.01
	323.15	0.0003	−0.0008	−0.0008	−0.0003	0.0009	0.01
$\Delta\sigma$/mN·m^{-1}	293.15	1.8689	−1.7683	−1.0406	0.9809		21
	303.15	1.0648	−3.3539	−1.1042	3.1945	0.3216	17
	313.15	−0.6510	−2.6916	0.4107	1.0221		26
	323.15	−1.8219	−3.1161	1.1114	2.4124		36

		Ethanol (1) + Benzyl Acetate (2) + Benzyl Alcohol (3)		
ΔQ_{123}	C_0	C_1	C_2	$\delta\cdot 10^3$
V^E/cm^3·mol^{-1}	0.1143	0.0190	−0.2449	4.4
$\Delta\eta$/mPa·s	−1.7728	2.5025	1.2648	6.0
Δn_D	−0.0059	0.0040	0.0030	0.03
$\Delta\sigma$/mN·m^{-1}	2.3354	−1.2707	0.9149	48

where ΔQ_{123} refers to the ternary V^E/cm^3·mol^{-1}, $\Delta\eta$/mPa·s, Δn_D, or $\Delta\sigma$/mN·m^{-1} and ΔQ_{ij} is the binary contribution given by eq 8. The ternary term Δ_{123} uses the expression suggested by Cibulka:[22]

$$\Delta_{123} = C_0 + C_1x_1 + C_2x_2 \tag{10}$$

The ternary parameters, C_i, were determined with the optimization algorithm similar to that for the binary parameters, a_k. Estimated values of C_k and δ are also gathered in Table 8. The standard deviations (δ) are about 0.004 cm^3·mol^{-1}, 0.006 mPa·s, 0.00003, and 0.1 mN·m^{-1} for V^E, $\Delta\eta$, n_D, and $\Delta\sigma$, respectively.

The values of V^E, which are negative over the entire composition range, for the binary systems at T = (293.15, 303.15, 313.15, and 323.15) K are presented in Tables 3 to 5. The values of V^E becomes more negative from T = (293.15 to 323.15) K for ethanol + benzyl alcohol mixtures. However, with the remaining binary systems, V^E values are found to become less negative with the increase of temperature, indicating the positive contribution to the V^E values from the cleavage of the acetate−alcohol complexation is dominant for these mixtures. As illustrated in Figure 1 for T = 303.15 K, the V^E values of benzyl acetate + benzyl alcohol are larger in magnitude when compared with those of the ethanol + benzyl acetate or + benzyl alcohol, for which the V^E values are more negative, which may be due to the formation of weak molecule complexes. Alternately, the V^E values of ethanol + benzyl alcohol mixtures are more negative than those of the ethanol + benzyl acetate, which imply that a weaker interaction likely exists between ethanol and benzyl acetate molecules. The values of V^E (x = 0.5) vary from −0.610 cm^3·mol^{-1} to −0.021 cm^3·mol^{-1}. As shown in Tables 3 to 5, the V^E results at other temperatures essentially follow the same trend as that of T = 303.15 K.

The values of $\Delta\eta$ are negative over the entire mole fraction range for all binary systems (Tables 3 to 5). A more efficient packing in the pure liquids than in the mixtures is perhaps the major contribution to negative $\Delta\eta$ values. The $\Delta\eta$ values are found to increase with a rise in temperature. The $\Delta\eta$ values are also graphically represented as a function of mole fraction for these three binary systems at T = 303.15 K in Figure 2. It is observed that the values of $\Delta\eta$ (x = 0.5) show the order as: benzyl acetate + benzyl alcohol < ethanol + benzyl alcohol < ethanol + benzyl acetate < 0. The values of $\Delta\eta(x = 0.5)$ vary from −0.776 mPa·s to −0.175 mPa·s. The same order in $\Delta\eta(x = 0.5)$ can also be found for the other temperatures. The viscosity behavior may imply an easier accommodation of the ethanol molecules in the mixture with benzyl acetate than in those with benzyl alcohol. The largest negative values of $\Delta\eta$ for the binary mixtures of benzyl acetate with benzyl alcohol are probably due to a more steric obstacle to this accommodation.

The calculated results of V^E and $\Delta\eta$ for the ternary system (ethanol + benzyl acetate + benzyl alcohol) at T = 303.15 K are presented in Table 6. The curves of constant V^E and $\Delta\eta$ at T = 303.15 K for the ternary mixtures were calculated from eqs 8 to 10 and plotted in Figures 3 and 4, respectively. As can be expected from the behavior of binary mixtures, the values of ternary V^E and $\Delta\eta$ are negative at all compositions. The minimum V^E value is near the ethanol + benzyl alcohol side at $x \approx$ 0.60 of ethanol, and the minimum $\Delta\eta$ value is near the benzyl acetate + benzyl alcohol side at $x \approx$ 0.40 of benzyl acetate.

■ CONCLUSIONS

This paper reports the experimental data of density (ρ), viscosity (η), refractive index (n_D), and surface tension (σ) for the ternary system (ethanol + benzyl acetate + benzyl alcohol) at T = 303.15 K and its constituent binary systems (ethanol + benzyl acetate, ethanol + benzyl alcohol, and benzyl acetate + benzyl alcohol) at T = (293.15, 303.15, 313.15, and 323.15) K. Increasing temperatures from (293.15 to 323.15) K decreases the values of ρ, η, n_D, and σ for binary mixtures. The experimental ρ, η, n_D, and σ of pure components are correlated in terms of temperature with reasonably small deviations.

The calculated excess molar volumes (V^E), deviations in viscosity ($\Delta\eta$), deviations in refractive index (Δn_D), and deviations in surface tension ($\Delta\sigma$) were correlated satisfactorily using the Redlich−Kister equation and the Cibulka equation. The values of binary V^E are negative, but some small positive values are observed for benzyl acetate + benzyl alcohol in the region of high mole fractions of benzyl acetate at T = (313.15 and 323.15) K. The values of V^E for the ternary system of ethanol + benzyl acetate + benzyl alcohol are negative at all compositions. The predominant contribution to these excess values is likely from the breaking of the hydrogen bonding between alcohol molecules. The values of $\Delta\eta$ are negative at all compositions for both binary and ternary systems. These values suggest that the interstitial accommodation between unlike molecules is not an easy process in the mixtures analyzed.

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Funding

The authors wish to extend their deep gratitude for the support by the National Science Council of Republic of China under grant NSC 95-2214-E-126-010-MY3.

Notes

The authors declare no competing financial interest.

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