Measurements of Density and Viscosity of Binary Mixtures of Several Flavor Compounds with 1-Butanol and 1-Pentanol at 293.15 K, 303.15 K, 313.15 K, and 323.15 K

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Density and viscosity for binary mixtures of four flavor compounds (benzyl acetate, 2-ethylhexyl acetate, benzaldehyde, and pentyl acetate) with 1-butanol and 1-pentanol over the whole composition range have been measured at four different temperatures (293.15, 303.15, 313.15, and 323.15 K) and atmospheric pressure. The excess molar volume (V^E) and viscosity deviations ($\Delta\eta_L$) were calculated and fitted to a Redlich−Kister type polynomial relation.

Introduction

The physical properties of a binary mixture such as density and viscosity are important from practical and theoretical points of view, to understand liquid theory. These properties are extremely useful for design of many types of transport and process equipment in chemical industries. A large amount of experiments[1−10] have been conducted to measure the densities and viscosities of liquid mixtures; however, reliable density and viscosity data over a wide range of composition and temperature for different systems are still needed.

Benzyl acetate, 2-ethylhexyl acetate, benzaldehyde, and pentyl acetate are important compounds in process manufacturing of the flavor and fragrance industries. To our knowledge, the density and viscosity data of these compounds in a binary mixture with 1-butanol and 1-pentanol at different temperatures and compositions have not been studied.

In this article we report our experimental data of the densities and viscosities of the binary mixtures of the above compounds at 293.15 K, 303.15 K, 313.15 K, and 323.15 K. From these data, the excess molar volume and the viscosity deviations were also calculated.

Experimental Section

Materials. High-purity flavor compounds (benzyl acetate, 2-ethylhexyl acetate, benzaldehyde, and *n*-amyl acetate), 1-butanol, and 1-pentanol were obtained from Merck KgaA, Germany. The purity of all compounds was assessed by gas chromatography (Shimadzu, GC-17A) using a flame ionization detector with a DB-5 column. The purities of all compounds are better than 98% for benzaldehyde, 2-ethylhexyl acetate, and pentyl acetate, and better than 99% for benzyl acetate, 1-butanol, and 1-pentanol, and no further purification was made.

Table 1. Comparison of Properties of Pure Liquids with Literature Data

		ρ_L/(g·cm^{-3})		η_L/(mPa·s)	
compound	T/K	exp	lit.	exp	lit.
benzyl acetate	293.15	1.054 93		2.323	
	303.15	1.048 17	1.0482[12]	1.838	
	313.15	1.041 41		1.487	
	323.15	1.034 65		1.230	
2-ethylhexyl acetate	293.15	0.873 52	0.8718[12]	1.471	1.500[12]
	303.15	0.864 37		1.234	
	313.15	0.855 09		1.051	
	323.15	0.846 07		0.906	
benzaldehyde	293.15	1.044 37	1.04463[12] 1.04470[13]	1.397	
	303.15	1.037 81		1.278	
	313.15	1.029 91		1.170	
	323.15	1.020 23		1.072	
pentyl acetate	293.15	0.876 67	0.8766[12]	0.931	0.924[12] 0.975[14]
	303.15	0.866 98		0.805	
	313.15	0.857 28		0.676	
	323.15	0.847 59		0.552	
1-butanol	293.15	0.809 13	0.80956[12]	2.864	
	303.15	0.805 54	0.80201[5]	2.273	2.271[12] 2.271[5]
	313.15	0.794 32	0.79432[5]	1.681	1.692[5]
	323.15	0.786 70		1.090	
1-pentanol	293.15	0.814 12	0.8144[12]	4.109	4.400[14]
	303.15	0.807 11	0.8072[12]	2.933	2.909[12] 3.202[14]
	313.15	0.799 78	0.800[12]	2.299	2.422[14]
	323.15	0.792 66		1.304	

Measurements. The binary mixture samples were prepared by mass in airtight stoppered glass bottles using a Mettler Toledo AE 240 balance with an uncertainty of $\pm 10^{-5}$ g. The mole fraction uncertainty for each binary mixture is estimated to be ±0.01%.

Densities of pure liquids and binary liquid mixtures were measured at 293.15 K, 303.15 K, 313.15 K, and 323.15 K

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Table 2. Experimental Density (ρ_L), Viscosity (η_L), Excess Molar Volume (V^E), and Viscosity Deviation ($\Delta\eta_L$) for Binary Mixtures of Benzyl Acetate (1) + 1-Butanol (2) at 293.15 K, 303.15 K, 313.15 K, and 323.15 K

x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)	x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)
				293.15 K					
0.0000	0.809 13	2.864	0.0000	0.0000	0.5973	0.975 89	2.527	0.5830	−0.0139
0.1023	0.843 09	2.803	0.3467	−0.0057	0.7048	0.999 52	2.471	0.4111	−0.0117
0.1976	0.871 68	2.748	0.6390	−0.0091	0.8005	1.019 00	2.422	0.2541	−0.0089
0.3075	0.902 89	2.685	0.7825	−0.0126	0.8914	1.036 13	2.376	0.1229	−0.0058
0.4014	0.928 03	2.633	0.7881	−0.0138	1.0000	1.054 93	2.323	0.0000	0.0000
0.5022	0.953 43	2.578	0.7091	−0.0143					
				303.15 K					
0.0000	0.805 54	2.273	0.0000	0.0000	0.5973	0.971 13	2.002	0.4707	−0.0112
0.1023	0.839 66	2.224	0.2832	−0.0045	0.7048	0.994 36	1.957	0.3066	−0.0094
0.1976	0.867 43	2.180	0.6311	−0.0070	0.8005	1.013 37	1.918	0.1738	−0.0068
0.3075	0.898 67	2.129	0.7258	−0.0102	0.8914	1.029 97	1.881	0.0793	−0.0042
0.4014	0.923 73	2.087	0.7001	−0.0114	1.0000	1.048 17	1.838	0.0000	0.0000
0.5022	0.948 94	2.043	0.6022	−0.0115					
				313.15 K					
0.0000	0.794 32	1.681	0.0000	0.0000	0.5973	0.964 55	1.562	0.2316	−0.0031
0.1023	0.828 97	1.660	0.2791	−0.0012	0.7048	0.987 95	1.542	0.1008	−0.0023
0.1976	0.858 63	1.641	0.4578	−0.0017	0.8005	1.006 96	1.524	0.0181	−0.0017
0.3075	0.890 73	1.619	0.5069	−0.0023	0.8914	1.023 44	1.507	−0.0117	−0.0011
0.4014	0.916 37	1.600	0.4587	−0.0031	1.0000	1.041 41	1.487	0.0000	0.0000
0.5022	0.942 06	1.581	0.3525	−0.0026					
				323.15 K					
0.0000	0.786 70	1.090	0.0000	0.0000	0.5973	0.958 05	1.172	0.1457	−0.0016
0.1023	0.822 47	1.104	0.1522	−0.0003	0.7048	0.981 45	1.187	0.0262	−0.0017
0.1976	0.852 13	1.116	0.3383	−0.0017	0.8005	1.000 46	1.201	−0.0454	−0.0011
0.3075	0.884 23	1.131	0.3960	−0.0020	0.8914	1.016 93	1.214	−0.0634	−0.0008
0.4014	0.909 87	1.144	0.3553	−0.0022	1.0000	1.034 65	1.230	0.0000	0.0000
0.5022	0.935 56	1.158	0.2577	−0.0023					

Table 3. Experimental Density (ρ_L), Viscosity (η_L), Excess Molar Volume (V^E), and Viscosity Deviation ($\Delta\eta_L$) for Binary Mixtures of 2-Ethylhexyl Acetate (1) + 1-Butanol (2) at 293.15 K, 303.15 K, 313.15 K, and 323.15 K

x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)	x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)
				293.15 K					
0.0000	0.809 13	2.864	0.0000	0.0000	0.6078	0.856 56	1.910	0.3839	−0.1073
0.0991	0.819 41	2.681	0.2552	−0.0449	0.7049	0.861 67	1.791	0.2634	−0.0911
0.2017	0.828 31	2.504	0.4777	−0.0790	0.8061	0.866 32	1.674	0.1486	−0.0671
0.2984	0.836 04	2.344	0.5694	−0.1043	0.9005	0.870 04	1.572	0.0722	−0.0376
0.4115	0.844 29	2.177	0.5645	−0.1138	1.0000	0.873 52	1.471	0.0000	0.0000
0.5002	0.850 16	2.052	0.5008	−0.1152					
				303.15 K					
0.0000	0.805 54	2.273	0.0000	0.0000	0.6078	0.849 72	1.568	0.2121	−0.0735
0.0991	0.815 32	2.139	0.1938	−0.0310	0.7049	0.854 05	1.478	0.1552	−0.0626
0.2017	0.824 10	2.010	0.3099	−0.0534	0.8061	0.858 05	1.389	0.0914	−0.0465
0.2984	0.831 17	1.894	0.3848	−0.0689	0.9005	0.861 35	1.311	0.0360	−0.0264
0.4115	0.838 65	1.768	0.3772	−0.0775	1.0000	0.864 37	1.234	0.0000	0.0000
0.5002	0.843 91	1.675	0.3259	−0.0783					
				313.15 K					
0.0000	0.794 32	1.681	0.0000	0.0000	0.6078	0.840 61	1.264	0.0939	−0.0341
0.0991	0.806 11	1.605	−0.0165	−0.0135	0.7049	0.845 15	1.207	0.0140	−0.0299
0.2017	0.814 53	1.529	0.1751	−0.0249	0.8061	0.849 17	1.151	−0.0366	−0.0222
0.2984	0.821 78	1.461	0.2490	−0.0320	0.9005	0.852 27	1.101	−0.0311	−0.0127
0.4115	0.829 44	1.386	0.2384	−0.0358	1.0000	0.855 09	1.051	0.0000	0.0000
0.5002	0.834 81	1.329	0.1842	−0.0369					
				323.15 K					
0.0000	0.786 70	1.090	0.0000	0.0000	0.6078	0.832 77	0.974	−0.0678	−0.0042
0.0991	0.798 78	1.070	−0.0891	−0.0018	0.7049	0.837 19	0.957	−0.1565	−0.0033
0.2017	0.806 85	1.050	0.1179	−0.0029	0.8061	0.840 99	0.939	−0.1879	−0.0027
0.2984	0.814 02	1.031	0.1736	−0.0041	0.9005	0.843 80	0.923	−0.1411	−0.0013
0.4115	0.821 52	1.010	0.1537	−0.0043	1.0000	0.846 07	0.906	0.0000	0.0000
0.5002	0.826 99	0.994	0.0555	−0.0039					

with a Mettler Toledo density meter (type DE50). The precision in the density measurement is estimated to be better than 10^{-5} g·cm^{-3}. Prior to use, the density meter was calibrated with double-distilled water. The temperature of the measuring cell was maintained using Julabo refrigerated and heating circulators (model F12-MD) with stability up to ±0.01 K.

Viscosities of pure liquids and binary liquids were measured by an automated microviscosimeter Anton Paar type AMVn. The accuracy in the viscosity measurement was estimated as better than 0.004 mPa·s. More details about the viscosity measurements are given elsewhere.[11]

All measurements described above were performed at least three times, and the results were averaged to give the final values. A comparison between the experimental results of density and viscosity of pure liquids and those from the literature is shown in Table 1. From this table, it can be seen that the experimental values of density and

Table 4. Experimental Density (ρ_L), Viscosity (η_L), Excess Molar Volume (V^E), and Viscosity Deviation ($\Delta\eta_L$) for Binary Mixtures of Benzaldehyde (1) + 1-Butanol (2) at 293.15 K, 303.15 K, 313.15 K, and 323.15 K

x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)	x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)
				293.15 K					
0.0000	0.809 13	2.864	0.0000	0.0000	0.6014	0.949 70	1.860	0.6871	−0.1217
0.1021	0.832 93	2.662	0.2834	−0.0522	0.6982	0.972 65	1.735	0.5835	−0.1047
0.2004	0.855 71	2.480	0.5024	−0.0900	0.8044	0.997 94	1.608	0.4129	−0.0759
0.3089	0.880 97	2.294	0.6593	−0.1168	0.9027	1.021 46	1.498	0.2045	−0.0417
0.4057	0.903 62	2.140	0.7284	−0.1288	1.0000	1.044 37	1.397	0.0000	0.0000
0.4992	0.925 58	2.001	0.7384	−0.1307					
				303.15 K					
0.0000	0.805 54	2.273	0.0000	0.0000	0.6014	0.945 50	1.608	0.5748	−0.0666
0.1021	0.829 42	2.143	0.2444	−0.0284	0.6982	0.967 99	1.521	0.4893	−0.0573
0.2004	0.852 28	2.025	0.4259	−0.0486	0.8044	0.992 66	1.430	0.3486	−0.0426
0.3089	0.877 51	1.903	0.5547	−0.0626	0.9027	1.015 49	1.352	0.1779	−0.0228
0.4057	0.900 01	1.799	0.6119	−0.0703	1.0000	1.037 81	1.278	0.0000	0.0000
0.4992	0.921 74	1.705	0.6188	−0.0713					
				313.15 K					
0.0000	0.794 32	1.681	0.0000	0.0000	0.6014	0.937 66	1.352	0.4107	−0.0217
0.1021	0.819 15	1.620	0.1671	−0.0088	0.6982	0.960 28	1.305	0.3495	−0.0192
0.2004	0.842 72	1.563	0.3015	−0.0156	0.8044	0.984 97	1.256	0.2489	−0.0139
0.3089	0.868 60	1.503	0.3962	−0.0202	0.9027	1.007 70	1.212	0.1275	−0.0077
0.4057	0.891 57	1.451	0.4374	−0.0227	1.0000	1.029 91	1.170	0.0000	0.0000
0.4992	0.913 65	1.403	0.4419	−0.0229					
				323.15 K					
0.0000	0.786 70	1.090	0.0000	0.0000	0.6014	0.930 33	1.079	0.2470	−0.0002
0.1021	0.811 96	1.088	0.0923	−0.0002	0.6982	0.952 57	1.077	0.2072	−0.0004
0.2004	0.835 75	1.086	0.1798	−0.0004	0.8044	0.976 71	1.075	0.1431	−0.0005
0.3089	0.861 73	1.084	0.2406	−0.0005	0.9027	0.998 80	1.074	0.0679	0.0002
0.4057	0.884 66	1.082	0.2667	−0.0007	1.0000	1.020 23	1.072	0.0000	0.000
0.4992	0.906 60	1.081	0.2680	−0.0006					

Table 5. Experimental Density (ρ_L), Viscosity (η_L), Excess Molar Volume (V^E), and Viscosity Deviation ($\Delta\eta_L$) for Binary Mixtures of Pentyl Acetate (1) + 1-Butanol (2) at 293.15 K, 303.15 K, 313.15 K, and 323.15 K

x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)	x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)
				293.15 K					
0.0000	0.809 13	2.864	0.0000	0.0000	0.6103	0.853 71	1.443	0.5733	−0.2413
0.1138	0.818 31	2.520	0.2945	−0.1240	0.7064	0.859 74	1.295	0.4824	−0.2035
0.2047	0.825 32	2.275	0.4621	−0.1933	0.8088	0.865 89	1.154	0.3471	−0.1466
0.3089	0.833 06	2.024	0.5828	−0.2429	0.9025	0.871 25	1.039	0.1969	−0.0805
0.4008	0.839 63	1.825	0.6317	−0.2643	1.0000	0.876 67	0.931	0.0000	0.0000
0.5000	0.846 45	1.633	0.6314	−0.2645					
				303.15 K					
0.0000	0.805 54	2.273	0.0000	0.0000	0.6103	0.846 63	1.206	0.4624	−0.1711
0.1138	0.814 12	2.020	0.2501	−0.0859	0.7064	0.852 07	1.092	0.3809	−0.1440
0.2047	0.820 62	1.838	0.3917	−0.1345	0.8088	0.857 57	0.982	0.2652	−0.1037
0.3089	0.827 77	1.649	0.4894	−0.1705	0.9025	0.862 33	0.891	0.1399	−0.0571
0.4008	0.833 81	1.499	0.5249	−0.1856	1.0000	0.866 98	0.805	0.0000	0.0000
0.5000	0.840 04	1.353	0.5183	−0.1860					
				313.15 K					
0.0000	0.794 32	1.681	0.0000	0.0000	0.6103	0.837 31	0.964	0.3433	−0.1036
0.1138	0.803 68	1.515	0.1895	−0.0516	0.7064	0.842 76	0.883	0.2735	−0.0881
0.2047	0.810 52	1.395	0.3101	−0.0803	0.8088	0.848 19	0.805	0.1831	−0.0632
0.3089	0.817 99	1.269	0.3870	−0.1016	0.9025	0.852 82	0.739	0.0927	−0.0350
0.4008	0.824 24	1.167	0.4101	−0.1112	1.0000	0.857 28	0.676	0.0000	0.0000
0.5000	0.830 63	1.066	0.3966	−0.1125					
				323.15 K					
0.0000	0.786 70	1.090	0.0000	0.0000	0.6103	0.829 07	0.720	0.2175	−0.0417
0.1138	0.795 96	1.009	0.1624	−0.0198	0.7064	0.834 26	0.674	0.1566	−0.0360
0.2047	0.802 82	0.948	0.2488	−0.0319	0.8088	0.839 34	0.629	0.0913	−0.0259
0.3089	0.810 24	0.883	0.2953	−0.0408	0.9025	0.843 59	0.590	0.0378	−0.0145
0.4008	0.816 40	0.830	0.2981	−0.0444	1.0000	0.847 59	0.552	0.0000	0.0000
0.5000	0.822 64	0.776	0.2711	−0.0450					

viscosity are generally in agreement with those from the literature.[5,11−13]

Results and Discussion

The density and viscosity data of various binary mixtures at 293.15 K, 303.15 K, 313.15 K, and 323.15 K are given in Tables 2−9. The values of excess molar volume, V^E, and viscosity deviation, $\Delta\eta_L$, were determined using the equations

$$V^E = \frac{x_1 M_1 + x_2 M_2}{\rho_L} - (x_1 V_1 + x_2 V_2) \tag{1}$$

$$\Delta\eta_L = \eta_L - (x_1 \eta_{L1} + x_2 \eta_{L2}) \tag{2}$$

where ρ_L and η_L are the density and viscosity of the mixture, respectively, and x_1, V_1, M_1, η_{L1}, x_2, V_2, M_2, and η_{L2} are the mole fraction, molar volume, molecular weight, and viscosity of pure compounds 1 and 2, respectively. The

Table 6. Experimental Density (ρ_L), Viscosity (η_L), Excess Molar Volume (V^E), and Viscosity Deviation ($\Delta\eta_L$) for Binary Mixtures of Benzyl Acetate (1) + 1-Pentanol (2) at 293.15 K, 303.15 K, 313.15 K, and 323.15 K

x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)	x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)
				293.15 K					
0.0000	0.814 12	4.109	0.0000	0.0000	0.6057	0.969 38	2.909	0.8018	−0.1182
0.1074	0.844 03	3.865	0.4106	−0.0522	0.7115	0.993 46	2.738	0.6529	−0.1003
0.2083	0.871 00	3.649	0.6886	−0.0879	0.8097	1.015 02	2.589	0.4719	−0.0739
0.2988	0.894 51	3.465	0.8353	−0.1103	0.9004	1.034 25	2.459	0.2778	−0.0419
0.4051	0.921 29	3.261	0.9054	−0.1245	1.0000	1.054 93	2.323	0.0000	0.0000
0.5012	0.944 72	3.087	0.8903	−0.1269					
				303.15 K					
0.0000	0.807 11	2.933	0.0000	0.0000	0.6057	0.963 61	2.210	0.6515	−0.0598
0.1074	0.837 40	2.789	0.3621	−0.0264	0.7115	0.987 63	2.103	0.5143	−0.0509
0.2083	0.864 69	2.661	0.5999	−0.0439	0.8097	1.009 07	2.009	0.3532	−0.0374
0.2988	0.888 42	2.551	0.7194	−0.0548	0.9004	1.028 12	1.926	0.1874	−0.0211
0.4051	0.915 39	2.427	0.7668	−0.0624	1.0000	1.048 17	1.838	0.0000	0.0000
0.5012	0.938 92	2.321	0.7409	−0.0632					
				313.15 K					
0.0000	0.799 78	2.299	0.0000	0.0000	0.6057	0.957 78	1.766	0.4877	−0.0412
0.1074	0.830 62	2.194	0.2932	−0.0178	0.7115	0.981 73	1.686	0.3687	−0.0353
0.2083	0.858 28	2.100	0.4870	−0.0299	0.8097	1.003 00	1.616	0.2395	−0.0255
0.2988	0.882 27	2.018	0.5770	−0.0384	0.9004	1.021 82	1.553	0.1137	−0.0149
0.4051	0.909 45	1.927	0.6030	−0.0431	1.0000	1.041 41	1.487	0.0000	0.0000
0.5012	0.933 08	1.848	0.5704	−0.0440					
				323.15 K					
0.0000	0.792 66	1.304	0.0000	0.0000	0.6057	0.951 93	1.259	0.3334	−0.0002
0.1074	0.824 09	1.296	0.2130	−0.0001	0.7115	0.975 70	1.251	0.2454	−0.0003
0.2083	0.852 09	1.288	0.3626	−0.0006	0.8097	0.996 71	1.244	0.1588	−0.0001
0.2988	0.876 29	1.281	0.4267	−0.0009	0.9004	1.015 21	1.237	0.0844	−0.0004
0.4051	0.903 61	1.274	0.4376	0.0000	1.0000	1.034 65	1.230	0.0000	0.0000
0.5012	0.927 29	1.266	0.4024	−0.0010					

Table 7. Experimental Density (ρ_L), Viscosity (η_L), Excess Molar Volume (V^E), and Viscosity Deviation ($\Delta\eta_L$) for Binary Mixtures of 2-Ethylhexyl Acetate (1) + 1-Pentanol (2) at 293.15 K, 303.15 K, 313.15 K, and 323.15 K

x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)	x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)
				293.15 K					
0.0000	0.814 12	4.109	0.0000	0.0000	0.6000	0.854 47	2.219	0.5928	−0.3072
0.1041	0.822 61	3.692	0.2694	−0.1424	0.7008	0.859 83	2.000	0.4782	−0.2603
0.2073	0.829 99	3.321	0.5030	−0.2411	0.8092	0.865 18	1.790	0.3191	−0.1843
0.3002	0.836 30	3.019	0.6253	−0.2981	0.9033	0.869 46	1.625	0.1654	−0.1011
0.4211	0.844 03	2.666	0.6804	−0.3321	1.0000	0.873 52	1.471	0.0000	0.0000
0.4987	0.848 70	2.462	0.6646	−0.3314					
				303.15 K					
0.0000	0.807 11	2.933	0.0000	0.0000	0.6000	0.847 24	1.745	0.3485	−0.1686
0.1041	0.815 47	2.680	0.2410	−0.0761	0.7008	0.852 29	1.599	0.2474	−0.1433
0.2073	0.823 03	2.451	0.4005	−0.1298	0.8092	0.857 18	1.456	0.1355	−0.1021
0.3002	0.829 41	2.262	0.4669	−0.1609	0.9033	0.860 99	1.342	0.0458	−0.0563
0.4211	0.837 11	2.037	0.4671	−0.1806	1.0000	0.864 37	1.234	0.0000	0.0000
0.4987	0.841 69	1.905	0.4288	−0.1807					
				313.15 K					
0.0000	0.799 78	2.299	0.0000	0.0000	0.6000	0.839 15	1.437	0.2277	−0.1132
0.1041	0.808 12	2.119	0.1998	−0.0501	0.7008	0.843 93	1.328	0.1418	−0.0964
0.2073	0.815 61	1.955	0.3258	−0.0853	0.8092	0.848 49	1.220	0.0608	−0.0691
0.3002	0.821 88	1.818	0.3698	−0.1064	0.9033	0.851 97	1.134	0.0135	−0.0377
0.4211	0.829 40	1.653	0.3491	−0.1205	1.0000	0.855 09	1.051	0.0000	0.0000
0.4987	0.833 83	1.556	0.3054	−0.1206					
				323.15 K					
0.0000	0.792 66	1.304	0.0000	0.0000	0.6000	0.830 95	1.048	0.1507	−0.0172
0.1041	0.800 72	1.255	0.1473	−0.0076	0.7008	0.835 52	1.010	0.0781	−0.0151
0.2073	0.808 07	1.209	0.2593	−0.0125	0.8092	0.839 85	0.971	0.0173	−0.0109
0.3002	0.814 21	1.169	0.2927	−0.0155	0.9033	0.843 10	0.938	−0.0009	−0.0065
0.4211	0.821 53	1.119	0.2663	−0.0174	1.0000	0.846 07	0.906	0.0000	0.0000
0.4987	0.825 82	1.087	0.2232	−0.0185					

excess molar volume and viscosity deviation values calculated from eqs 1 and 2 are also summarized in Tables 2−9.

The excess molar volume, V^E, and viscosity deviation, $\Delta\eta_L$, were fitted to the well-known Redlich−Kister[15] polynomial equation

$$V^E = x_1 x_2 \sum_{i=0}^{n} b_i (x_1 - x_2)^i \qquad (3)$$

or

$$\Delta\eta_L = x_1 x_2 \sum_{i=0}^{n} b_i (x_1 - x_2)^i \qquad (4)$$

where b_i are parameters and n is the number of polynomial coefficients or parameters. The parameters b_i were obtained by a least-squares method, and the standard error, σ,

Table 8. Experimental Density (ρ_L), Viscosity (η_L), Excess Molar Volume (V^E), and Viscosity Deviation ($\Delta\eta_L$) for Binary Mixtures of Benzaldehyde (1) + 1-Pentanol (2) at 293.15 K, 303.15 K, 313.15 K, and 323.15 K

x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)	x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)
				293.15 K					
0.0000	0.814 12	4.109	0.0000	0.0000	0.5990	0.941 64	2.153	0.7606	−0.3315
0.1001	0.833 44	3.688	0.3156	−0.1495	0.7004	0.966 31	1.930	0.6403	−0.2795
0.2014	0.853 64	3.307	0.5695	−0.2558	0.8063	0.993 04	1.722	0.4563	−0.2003
0.3028	0.874 77	2.964	0.7316	−0.3238	0.9052	1.018 88	1.547	0.2384	−0.1071
0.4151	0.899 22	2.626	0.8153	−0.3572	1.0000	1.044 37	1.397	0.0000	0.0000
0.5074	0.920 14	2.377	0.8156	−0.3559					
				303.15 K					
0.0000	0.807 11	2.933	0.0000	0.0000	0.5990	0.935 83	1.783	0.6509	−0.1587
0.1001	0.826 93	2.699	0.2547	−0.0683	0.7004	0.960 40	1.639	0.5502	−0.1348
0.2014	0.847 43	2.481	0.4769	−0.1187	0.8063	0.986 94	1.501	0.3951	−0.0976
0.3028	0.868 77	2.281	0.6204	−0.1509	0.9052	1.012 53	1.383	0.2105	−0.0519
0.4151	0.893 37	2.078	0.6949	−0.1680	1.0000	1.037 81	1.278	0.0000	0.0000
0.5074	0.914 34	1.924	0.6971	−0.1693					
				313.15 K					
0.0000	0.799 78	2.299	0.0000	0.0000	0.5990	0.929 68	1.534	0.4789	−0.0887
0.1001	0.819 89	2.149	0.2094	−0.0369	0.7004	0.953 99	1.432	0.4057	−0.0762
0.2014	0.840 86	2.007	0.3657	−0.0646	0.8063	0.980 11	1.334	0.2935	−0.0547
0.3028	0.862 52	1.874	0.4656	−0.0831	0.9052	1.005 16	1.247	0.1618	−0.0300
0.4151	0.887 31	1.737	0.5147	−0.0934	1.0000	1.029 91	1.170	0.0000	0.0000
0.5074	0.908 29	1.632	0.5146	−0.0941					
				323.15 K					
0.0000	0.792 66	1.304	0.0000	0.0000	0.5990	0.922 37	1.160	0.3395	−0.0050
0.1001	0.812 98	1.279	0.1531	−0.0018	0.7004	0.946 27	1.137	0.2858	−0.0045
0.2014	0.834 09	1.254	0.2640	−0.0033	0.8063	0.971 83	1.113	0.2057	−0.0039
0.3028	0.855 78	1.229	0.3340	−0.0048	0.9052	0.996 25	1.092	0.1120	−0.0020
0.4151	0.880 46	1.202	0.3682	−0.0057	1.0000	1.020 23	1.072	0.0000	0.0000
0.5074	0.901 26	1.181	0.3662	−0.0053					

Table 9. Experimental Density (ρ_L), Viscosity (η_L), Excess Molar Volume (V^E), and Viscosity Deviation ($\Delta\eta_L$) for Binary Mixtures of Pentyl Acetate (1) + 1-Pentanol (2) at 293.15 K, 303.15 K, 313.15 K, and 323.15 K

x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)	x_1	ρ_L/(g·cm^{-3})	η_L/(mPa·s)	V^E/(cm^3·mol^{-1})	$\Delta\eta_L$/(mPa·s)
				293.15 K					
0.0000	0.814 12	4.109	0.0000	0.0000	0.6044	0.853 55	1.675	0.4524	−0.5132
0.0982	0.821 07	3.552	0.1609	−0.2449	0.7081	0.859 80	1.436	0.3840	−0.4227
0.1951	0.827 54	3.076	0.3068	−0.4130	0.8063	0.865 59	1.241	0.2856	−0.3056
0.3024	0.834 56	2.623	0.4159	−0.5250	0.9007	0.871 04	1.079	0.1619	−0.1676
0.4009	0.840 88	2.266	0.4696	−0.5689	1.0000	0.876 67	0.931	0.0000	0.0000
0.5015	0.847 21	1.952	0.4815	−0.5632					
				303.15 K					
0.0000	0.807 11	2.933	0.0000	0.0000	0.6044	0.845 39	1.343	0.3614	−0.3038
0.0982	0.813 86	2.583	0.1456	−0.1410	0.7081	0.851 33	1.174	0.2987	−0.2521
0.1951	0.820 23	2.279	0.2636	−0.2388	0.8063	0.856 78	1.034	0.2150	−0.1832
0.3024	0.827 10	1.984	0.3481	−0.3054	0.9007	0.861 87	0.915	0.1128	−0.1013
0.4009	0.833 23	1.747	0.3872	−0.3329	1.0000	0.866 98	0.805	0.0000	0.0000
0.5015	0.839 33	1.534	0.3908	−0.3318					
				313.15 K					
0.0000	0.799 78	2.299	0.0000	0.0000	0.6044	0.837 04	1.097	0.2785	−0.2211
0.0982	0.806 39	2.039	0.1264	−0.1006	0.7081	0.842 66	0.966	0.2285	−0.1838
0.1951	0.812 68	1.811	0.2178	−0.1714	0.8063	0.847 77	0.857	0.1650	−0.1334
0.3024	0.819 40	1.588	0.2819	−0.2202	0.9007	0.852 49	0.763	0.0918	−0.0742
0.4009	0.825 37	1.407	0.3065	−0.2413	1.0000	0.857 28	0.676	0.0000	0.0000
0.5015	0.831 25	1.244	0.3048	−0.2411					
				323.15 K					
0.0000	0.792 66	1.304	0.0000	0.0000	0.6044	0.828 88	0.776	0.1731	−0.0735
0.0982	0.799 24	1.198	0.0868	−0.0322	0.7081	0.834 18	0.709	0.1327	−0.0625
0.1951	0.805 39	1.103	0.1554	−0.0543	0.8063	0.838 96	0.652	0.0852	−0.0457
0.3024	0.811 95	1.001	0.1957	−0.0756	0.9007	0.843 33	0.601	0.0353	−0.0257
0.4009	0.817 72	0.924	0.2075	−0.0785	1.0000	0.847 59	0.552	0.0000	0.0000
0.5015	0.823 36	0.847	0.1998	−0.0799					

between the experimental values and the calculated ones was estimated by

$$\sigma(V^E) = \left[\frac{\sum({V_{exp}}^E - {V_{cal}}^E)^2}{(N - n)}\right]^{0.5} \quad (5)$$

or

$$\sigma(\Delta\eta_L) = \left[\frac{\sum(\Delta\eta_{L,exp} - \Delta\eta_{L,cal})^2}{(N - n)}\right]^{0.5} \quad (6)$$

where N is the number of experimental data points. The values of b_i and σ are presented in Table 10. The uncertainties of the excess molar volumes and viscosity deviations are estimated to be ±0.0001 cm^3·mol^{-1} and ±0.0001 mPa·s, respectively.

Table 10. Parameters and Standard Deviation of Redlich–Kister Polynomial Equation

system		T/K	b_0	b_1	b_2	b_3	σ
benzyl acetate + 1-butanol	V^E/(cm^3·mol^{-1})	293.15	2.8750	−2.3231	−0.3526	1.0540	0.0112
		303.15	2.4711	−2.7990	−0.2987	1.8164	0.0292
		313.15	1.4324	−2.5193	0.1137	0.7538	0.0053
		323.15	1.0804	−2.4066	−0.6480	1.3601	0.0141
	$\Delta\eta_L$/(mPa·s)	293.15	−0.0573	0.0024	−0.0022	−0.0012	0.0002
		303.15	−0.0467	0.0024	0.0044	−0.0004	0.0003
		313.15	−0.0117	−0.0006	−0.0012	−0.0024	0.0001
		323.15	−0.0087	−0.0054	−0.0018	−0.0115	0.0004
2-ethylhexyl acetate + 1-butanol	V^E/(cm^3·mol^{-1})	293.15	2.0183	−1.9581	−0.2015	−0.9685	0.0059
		303.15	1.2761	−1.4900	−0.0056	0.7644	0.0103
		313.15	0.7882	−1.8028	−1.2685	2.4241	0.0200
		323.15	0.3073	−2.5451	−1.9316	3.1707	0.0268
	$\Delta\eta_L$/(mPa·s)	293.15	−0.4627	0.0679	−0.0009	−0.0295	0.0010
		303.15	−0.3139	0.0319	−0.0071	−0.0016	0.0007
		313.15	−0.1468	0.0136	−0.0027	−0.0108	0.0006
		323.15	−0.0171	0.0024	−0.0017	0.0000	0.0008
benzaldehyde + 1-butanol	V^E/(cm^3·mol^{-1})	293.15	2.9647	−0.3821	−0.2977	−0.1277	0.0042
		303.15	2.4801	−0.3414	−0.1540	−0.0785	0.0023
		313.15	1.7750	−0.2595	−0.1576	−0.0440	0.0025
		323.15	1.0823	−0.1965	−0.2311	0.0778	0.0031
	$\Delta\eta_L$/(mPa·s)	293.15	−0.5220	0.0679	−0.0007	−0.0115	0.0001
		303.15	−0.2844	−0.0284	−0.0023	0.0012	0.0001
		313.15	−0.0923	0.0067	−0.0009	−0.0013	0.0004
		323.15	−0.0014	0.0011	−0.0013	0.0000	0.0030
pentyl acetate + 1-butanol	V^E/(cm^3·mol^{-1})	293.15	2.5231	−0.5393	0.0801	0.1521	0.0010
		303.15	2.0755	−0.5774	−0.0319	0.0225	0.0009
		313.15	1.5920	−0.6520	−0.1505	0.2007	0.0023
		323.15	1.0904	−0.7967	−0.0733	−0.0752	0.0012
	$\Delta\eta_L$/(mPa·s)	293.15	−1.0581	0.2002	−0.0300	−0.0016	0.0002
		303.15	−0.7461	−0.1304	−0.0114	−0.0253	0.0001
		313.15	−0.4498	0.0635	−0.0085	0.00156	0.0003
		323.15	−0.1807	0.0237	−0.0030	−0.0042	0.0002
benzyl acetate + 1-pentanol	V^E/(cm^3·mol^{-1})	293.15	3.5610	−1.0633	0.1972	0.4508	0.0024
		303.15	2.9725	−1.1510	−0.0013	0.1255	0.0024
		313.15	2.2951	−1.1692	−0.1167	0.0577	0.0037
		323.15	1.6209	−1.0989	−0.0138	0.4303	0.0028
	$\Delta\eta_L$/(mPa·s)	293.15	−0.5071	0.0473	0.0000	−0.0017	0.0005
		303.15	−0.2541	0.0156	−0.0030	0.0134	0.0004
		313.15	−0.1764	0.0146	0.0023	−0.0039	0.0007
		323.15	−0.0019	0.0035	−0.0009	−0.0064	0.0001
2-rthylhexyl acetate + 1-pentanol	V^E/(cm^3·mol^{-1})	293.15	2.6679	−0.9567	−0.3364	0.4483	0.0051
		303.15	1.7210	−1.3035	−0.1739	0.0319	0.0032
		313.15	1.2238	−1.3838	−0.0695	0.2095	0.0019
		323.15	0.8958	−1.3709	−0.1289	0.5406	0.0035
	$\Delta\eta_L$/(mPa·s)	293.15	−1.3249	0.2226	−0.0280	0.0136	0.0001
		303.15	−0.7231	0.1039	−0.0121	0.0063	0.0003
		313.15	−0.4833	0.0567	−0.0015	0.0110	0.0003
		323.15	−0.0721	0.0013	−0.0061	0.0067	0.0004
benzaldehyde + 1-pentanol	V^E/(cm^3·mol^{-1})	293.15	3.2780	−0.5435	−0.1574	0.1295	0.0025
		303.15	2.8028	−0.4524	−0.1918	0.3162	0.0030
		313.15	2.0610	−0.3638	0.0576	0.1257	0.0009
		323.15	1.4672	−0.2874	0.0449	0.0596	0.0005
	$\Delta\eta_L$/(mPa·s)	293.15	−1.4277	0.2518	−0.0364	0.0078	0.0003
		303.15	−0.6778	0.0885	−0.0090	0.0120	0.0002
		313.15	−0.3775	0.0410	−0.0008	−0.0028	0.0003
		323.15	−0.0219	0.0032	−0.0009	−0.0119	0.0002
pentyl acetate + 1-pentanol	V^E/(cm^3·mol^{-1})	293.15	1.9325	−0.1828	−0.1412	0.2560	0.0021
		303.15	1.5700	−0.2518	−0.1432	0.0176	0.0017
		313.15	1.2214	−0.2898	0.0063	0.0572	0.0005
		323.15	0.8049	−0.3452	−0.1347	−0.0363	0.0021
	$\Delta\eta_L$/(mPa·s)	293.15	−2.2558	0.5465	−0.1010	0.0131	0.0002
		303.15	−1.3278	0.2820	−0.0527	0.0064	0.0001
		313.15	−0.9646	0.1939	−0.0251	−0.0034	0.0002
		323.15	−0.3208	0.0634	−0.0092	−0.0323	0.0014

From Tables 2−9, it can be seen that the V^E values are positive for almost all mixtures except for benzyl acetate + 1-butanol and 2-ethylhexyl acetate + 1-butanol at high mole fraction and temperature (313.15 K and 323.15 K). The positive V^E values result from breaking up of H-bonding in alcohols by flavor compounds and also the size of these molecules. The excess molar volumes decrease with increasing temperature. The $\Delta\eta_L$ values are negative for almost all mixtures and increase with increasing temperature. Very small viscosity deviations are observed for the systems benzaldehyde + 1-butanol and benzyl acetate + 1-pentanol at 323.15 K, indicating that at high temperature these systems are likely close to ideal systems. Figures 1 and 2 depict the excess molar volumes and viscosity deviations for all systems at 293.15 K. Figure 1 indicates that the V^E values of flavor compound + 1-pentanol systems are higher than those of flavor compound + 1-butanol systems except for pentyl acetate + 1-pentanol. As shown in Figure 2, the molecular size of the alkanol also affects the $\Delta\eta_L$ values at all concentration ranges of

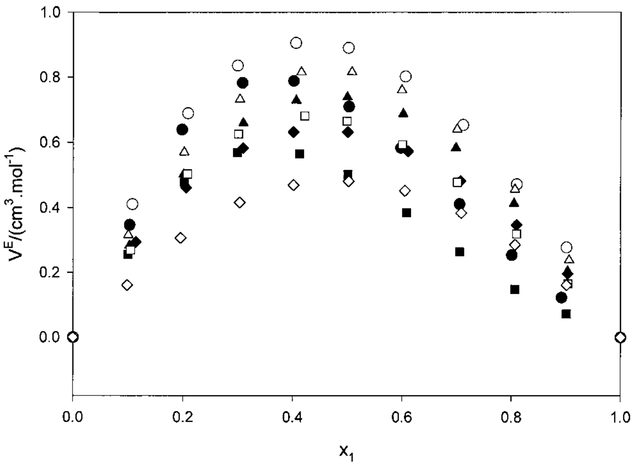

Figure 1. Excess molar volumes, V^E, at 293.15 K for (●) benzyl acetae (1) + 1-butanol (2), (■) 2-ethylhexyl acetate (1) + 1-butanol (2), (▲) benzaldehyde (1) + 1-butanol (2), (◆) pentyl acetate (1) + 1-butanol (2), (○) benzyl acetate (1) + 1-pentanol (2), (□) 2-ethylhexyl acetate (1) + 1-pentanol (2), (△) benzaldehyde (1) + 1-pentanol (2), and (◇) pentyl acetate (1) + 1-pentanol (2).

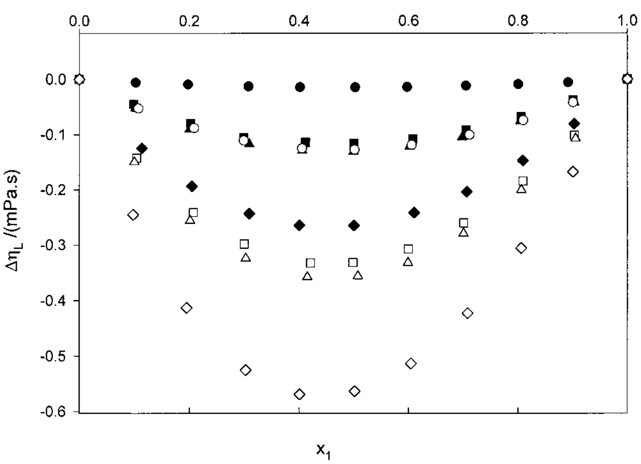

Figure 2. $\Delta\eta_L$ values at 293.15 K for (●) benzyl acetae (1) + 1-butanol (2), (■) 2-ethylhexyl acetate (1) + 1-butanol (2), (▲) benzaldehyde (1) + 1-butanol (2), (◆) pentyl acetate (1) + 1-butanol (2), (○) benzyl acetate (1) + 1-pentanol (2), (□) 2-ethylhexyl acetate (1) + 1-pentanol (2), (△) benzaldehyde (1) + 1-pentanol (2), and (◇) pentyl acetate (1) + 1-pentanol (2).

the mixtures; with the increase of alkanol size, the $\Delta\eta_L$ values of the mixtures decrease several times. The minima of the $\Delta\eta_L$ versus x_i curves located near $x_1 \approx 0.4-0.5$.

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