Systematic Determination of Densities and Speeds of Sound of Nitroethane + Isomers of Butanol in the Range (283.15−308.15) K

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Densities and speeds of sound were measured for nitroethane + 1-butanol, nitroethane + 2-butanol, and nitroethane + 2-methyl-1-propanol at atmospheric pressure and at 11 temperatures in the range (283.15−308.15) K over the whole composition range. The densimeter and sound analyzer Anton Paar DSA-48 was used for the measurements. These results are used to calculate excess molar volumes, excess isobaric thermal expansivities, and isentropic compressibilities. Results are discussed in terms of well-known effects in mixtures containing alcohols.

Introduction

During the last few years the thermodynamic properties of binary mixtures of alkane + alcohol have been studied extensively (Romaní et al.;[1] Heintz et al.;[2] Berro et al.[3]). Nevertheless, the mixtures containing a polar component without hydrogen bonds and an alcohol have not been studied so extensively, especially the temperature dependence of their thermodynamic properties.

The aim of this work is to provide experimental data on such mixtures, specifically, densities, speeds of sound, and derived magnitudes of systems containing nitroethane + alcohol. We report such data at atmospheric pressure in the temperature range (283.15−308.15) K, for nitroethane + 1-butanol, nitroethane + 2-butanol, and nitroethane + 2-methyl-1-propanol.

Experimental Section

Materials. Nitroethane (>97% mol) and 1-butanol (>99.8% mol) were supplied from Fluka, 2-methyl-1-propanol (>99.45% mol) was supplied from Sigma-Aldrich, and 2-butanol (99.45% mol) was from Aldrich. All chemicals were partially degassed and dried over Fluka type 0.4 nm molecular sieves. The purity of the products was checked by using gas chromatography (GC).

Apparatus and Procedure. Densities and speeds of sound of the pure components and of the binary mixtures were determined with a DSA-48 densimeter and sound analyzer from Anton Paar. This apparatus measures simultaneously the density using a vibrating tube and the sound velocity through ultrasonic pulses. The temperature was controlled through a solid-state thermostat that uses the Peltier effect. The precision in the temperature was ±0.005 K.

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This apparatus is connected to a personal computer through a RS-232 connection. Once the sample is introduced in the measuring cell, the user can make a program in order to get measurements at the desired temperatures. Later, these experimental data were filled in the nonvolatile memory of the computer. The precision is estimated to be about 2×10^{-5} for x, $\pm 1 \times 10^{-5}$ g·cm^{-3} for ρ, and ±0.02 m·s^{-1} for u. Calibration was done also automatically in the studied temperature range, using *n*-heptane (>99.8% mol) from Fluka and pure water (MilliQ). The densities of the pure water at several temperatures were obtained from Riddick et al.,[4] and those of *n*-heptane were obtained in a previous work[5] measuring them with two density standards supplied by the Deutscher Kalibrierdienst-Physikalisch Technische Bundesanstalt. The speeds of sound of water (only one standard is needed for this magnitude) were obtained from the work of Bilaniuk et al.[6,7]

Results and Discussion

Densities ρ of the pure liquids and their comparison with literature data are presented in Table 1. Isobaric thermal expansivities α at 298.15 K were calculated from analytical differentiation of the density fitting equation, and their values for the pure liquids are also given in Table 1 compared to the literature ones. Isentropic compressibilities κ_S of the pure liquids were calculated from the Laplace equation

$$\kappa_S = \frac{1}{\rho u^2} \tag{1}$$

where u is the speed of sound; the values are given in Table 2 along with literature data.

Densities and speeds of sound of the mixtures are presented in Tables 3 and 4, respectively. Density, speed of sound, and isentropic compressibility data were fitted

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Table 1. Densities, ρ, and Isobaric Thermal Expansivities, α, for the Pure Liquids at the Temperature T

component	T/K	this work	lit.	T/K	this work	lit.
			ρ/g·cm^{-3}			
nitroethane	283.15	1.062 78		298.15	1.044 70	1.046 40[4]
	286.15	1.059 16		301.15	1.041 07	
	288.15	1.056 74		303.15	1.038 59	1.038 70[4]
	291.15	1.054 34		306.15	1.034 87	
	293.15	1.050 74	1.050 57[4]	308.15	1.032 44	
	296.15	1.047 12				
1-butanol	283.15	0.817 04	0.817 02[2]	298.15	0.805 62	0.805 75[4]
	286.15	0.814 76		301.15	0.803 32	
	288.15	0.813 24		303.15	0.801 79	
	291.15	0.810 95		306.15	0.799 47	
	293.15	0.809 43	0.809 56[4]	308.15	0.797 93	
	296.15	0.807 15				
2-methyl-1propanol	283.15	0.809 27		298.15	0.797 77	0.797 8[4]
	286.15	0.806 98		301.15	0.795 45	
	288.15	0.805 44		303.15	0.793 87	
	291.15	0.803 16		306.15	0.791 49	
	293.15	0.801 62	0.801 6[4]	308.15	0.789 90	
	296.15	0.799 32				
2-butanol	283.15	0.814 48		298.15	0.802 39	0.802 41[4]
	286.15	0.812 10		301.15	0.799 89	
	288.15	0.810 51		303.15	0.798 19	
	291.15	0.808 10		306.15	0.795 60	
	293.15	0.806 48	0.806 52[4]	308.15	0.793 88	
	296.15	0.804 04				
			$\alpha/10^{-3}$ K^{-1}			
nitroethane	298.15	1.16	1.14[4]			
1-butanol	298.15	1.01	1.024[4]			
2-methyl-1propanol	298.15	0.96	0.95[4]			
2-butanol	298.15	0.95	0.948[4]			

Table 2. Speeds of Sound, u, and Isentropic Compressibilities, κ_S, for the Pure Liquids at the Temperature T

component	T/K	u/m·s^{-1}	κ_S/TPa^{-1}	T/K	u/m·s^{-1}	κ_S/TPa^{-1}	κ_S/TPa^{-1}
		this work			this work		lit.
nitroethane	283.15	1335.69	527.41	298.15	1275.99	587.91	
	286.15	1323.79	538.77	301.15	1264.14	601.08	
	288.15	1315.86	546.53	303.15	1256.32	610.04	
	291.15	1303.73	558.01	306.15	1244.67	623.74	
	293.15	1295.78	566.82	308.15	1237.44	632.54	
	296.15	1283.93	579.32				
1-butanol	283.15	1290.41	735.02	298.15	1238.99	808.60	
	286.15	1280.01	749.11	301.15	1228.82	824.39	
	288.15	1273.12	758.65	303.15	1222.08	835.10	
	291.15	1262.73	773.37	306.15	1212.10	851.38	
	293.15	1255.94	783.22	308.15	1205.79	861.97	866[4]
	296.15	1245.77	798.31				
2-methyl-1-propanol	283.15	1237.48	806.92	298.15	1186.72	890.07	
	286.15	1227.39	822.57	301.15	1176.75	907.86	
	288.15	1220.64	833.28	303.15	1170.08	920.07	
	291.15	1210.31	849.97	306.15	1160.15	938.70	
	293.15	1203.56	861.18	308.15	1153.86	950.87	950[4]
	296.15	1193.49	878.30				
2-butanol	283.15	1263.90	768.59	298.15	1210.43	850.62	848.4[8]
	286.15	1253.46	783.74	301.15	1199.66	868.67	
	288.15	1246.38	794.22	303.15	1192.47	881.05	
	291.15	1235.55	810.61	306.15	1181.67	900.15	
	293.15	1228.38	821.75	308.15	1174.89	912.54	
	296.15	1217.66	838.82				

simultaneously as a function of composition and temperature according to the expression

$$Y = \sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij} 10^{1-j} x^{i-1} (\mathrm{T}/K - T_0)^{j-1} \qquad (2)$$

where x is the nitroethane mole fraction, T is the absolute temperature, $T_0 = 280.15$, and Y can be the density ρ/g·cm^{-3}, the speed of sound u/m·s^{-1}, or the isentropic compressibility κ_S/TPa^{-1}. The coefficients A_{ij} were obtained through Marquardt's algorithm (Marquardt[9]) and are listed in Tables 5−7, together with the standard deviations s.

Excess molar volumes v^E and excess isobaric thermal expansivities α^E for all systems were calculated from measured data. The precision of those excess quantities is a good measure of that of the primary data. We adopted the ideality criterion of Benson and Kiyohara,[10] which is the most frequent choice for this purpose:

$$v^E = \frac{xM_1 + (1-x)M_2}{\rho} - \left(x\frac{M_1}{\rho_1} + (1-x)\frac{M_2}{\rho_2} \right) \qquad (3)$$

$$\alpha^E = \alpha - (\phi\alpha_1 + (1-\phi)\alpha_2) \qquad (4)$$

Here x is the mole fraction of component 1, M is the

Table 3. Densities, ρ, for the Mixtures in the Temperature Range (283.15−308.15) K

	ρ/g·cm^{-3}										
x	283.15 K	286.15 K	288.15 K	291.15 K	293.15 K	296.15 K	298.15 K	301.15 K	303.15 K	306.15 K	308.15 K
					x Nitroethane + (1 − x) 1-Butanol						
0.055 30	0.827 67	0.825 29	0.823 72	0.821 35	0.819 78	0.817 41	0.815 82	0.813 44	0.811 85	0.809 43	0.807 81
0.103 38	0.837 10	0.834 66	0.833 04	0.830 62	0.828 99	0.826 55	0.824 90	0.822 46	0.820 79	0.818 28	0.816 62
0.204 27	0.857 35	0.854 77	0.853 07	0.850 51	0.848 79	0.846 21	0.844 48	0.841 89	0.840 13	0.837 46	0.835 72
0.358 52	0.890 35	0.887 57	0.885 71	0.882 94	0.881 09	0.878 28	0.876 42	0.873 61	0.871 70	0.868 82	0.866 93
0.394 95	0.898 41	0.895 58	0.893 69	0.890 85	0.888 96	0.886 11	0.884 20	0.881 34	0.879 43	0.876 51	0.874 57
0.502 34	0.923 46	0.920 48	0.918 50	0.915 53	0.913 55	0.910 56	0.908 56	0.905 56	0.903 51	0.900 43	0.898 40
0.582 56	0.943 06	0.939 96	0.937 89	0.934 81	0.932 75	0.929 65	0.927 58	0.924 46	0.922 37	0.919 20	0.917 08
0.652 34	0.960 86	0.957 67	0.955 56	0.952 39	0.950 28	0.947 08	0.944 95	0.941 75	0.939 57	0.936 27	0.934 12
0.800 40	1.001 21	0.997 83	0.995 58	0.992 21	0.989 97	0.986 56	0.984 32	0.980 91	0.978 60	0.975 12	0.972 82
0.897 94	1.030 01	1.026 50	1.024 18	1.020 68	1.018 35	1.014 84	1.012 49	1.009 00	1.006 59	1.002 98	1.000 63
					x Nitroethane + (1 − x) 2-Methyl-1-propanol						
0.055 13	0.820 42	0.818 03	0.816 44	0.814 06	0.812 45	0.810 04	0.808 42	0.805 99	0.804 34	0.801 85	0.800 21
0.103 94	0.830 20	0.827 73	0.826 10	0.823 63	0.821 98	0.819 49	0.817 83	0.815 33	0.813 63	0.811 06	0.809 36
0.207 66	0.851 76	0.849 14	0.847 40	0.844 79	0.843 05	0.840 41	0.838 64	0.835 99	0.834 18	0.831 45	0.829 64
0.307 31	0.873 36	0.870 62	0.868 78	0.866 04	0.864 19	0.861 41	0.859 54	0.856 75	0.854 85	0.851 98	0.850 09
0.455 16	0.907 55	0.904 61	0.902 65	0.899 70	0.897 74	0.894 76	0.892 78	0.889 79	0.887 75	0.884 69	0.882 67
0.508 06	0.920 50	0.917 49	0.915 48	0.912 46	0.910 45	0.907 41	0.905 38	0.902 33	0.900 26	0.897 12	0.895 07
0.549 55	0.930 92	0.927 85	0.925 80	0.922 73	0.920 66	0.917 56	0.915 48	0.912 37	0.910 24	0.907 05	0.904 94
0.618 64	0.948 76	0.945 60	0.943 50	0.940 34	0.938 23	0.935 04	0.932 91	0.929 72	0.927 55	0.924 26	0.922 10
0.702 29	0.971 31	0.968 03	0.965 85	0.962 59	0.960 41	0.957 11	0.954 92	0.951 60	0.949 35	0.945 96	0.943 73
0.803 99	1.000 21	0.996 81	0.994 54	0.991 14	0.988 89	0.985 46	0.983 19	0.979 77	0.977 43	0.973 92	0.971 60
0.902 79	1.030 43	1.026 91	1.024 59	1.021 08	1.018 74	1.015 22	1.012 88	1.009 35	1.006 95	1.003 33	1.000 96
0.954 20	1.047 25	1.043 67	1.041 30	1.037 74	1.035 37	1.031 78	1.029 41	1.025 83	1.023 38	1.019 70	1.017 30
					x Nitroethane + (1 − x) 2-Butanol						
0.059 89	0.825 70	0.823 19	0.821 51	0.818 98	0.817 27	0.814 69	0.812 95	0.810 35	0.808 56	0.805 86	0.804 07
0.097 71	0.832 84	0.830 26	0.828 54	0.825 95	0.824 19	0.821 56	0.819 78	0.817 11	0.815 29	0.812 53	0.810 71
0.206 01	0.854 26	0.851 51	0.849 68	0.846 93	0.845 08	0.842 28	0.840 40	0.837 59	0.835 67	0.832 76	0.830 83
0.309 19	0.875 90	0.873 01	0.871 09	0.868 19	0.866 26	0.863 31	0.861 35	0.858 39	0.856 38	0.853 34	0.851 32
0.352 70	0.885 42	0.882 48	0.880 53	0.877 57	0.875 60	0.872 60	0.870 60	0.867 59	0.865 54	0.862 45	0.860 40
0.404 90	0.897 17	0.894 17	0.892 17	0.889 15	0.887 14	0.884 09	0.882 05	0.878 98	0.876 89	0.873 74	0.871 65
0.496 74	0.918 85	0.915 72	0.913 63	0.910 51	0.908 41	0.905 25	0.903 14	0.899 97	0.897 80	0.894 54	0.892 39
0.515 21	0.923 31	0.920 17	0.918 07	0.914 93	0.912 82	0.909 64	0.907 53	0.904 34	0.902 17	0.898 88	0.896 73
0.517 54	0.923 87	0.920 71	0.918 61	0.915 45	0.913 35	0.910 16	0.908 03	0.904 84	0.902 66	0.899 38	0.897 21
0.615 30	0.948 30	0.945 04	0.942 87	0.939 61	0.937 43	0.934 15	0.931 95	0.928 65	0.926 40	0.923 02	0.920 79
0.625 69	0.951 01	0.947 74	0.945 56	0.942 30	0.940 11	0.936 82	0.934 62	0.931 30	0.929 05	0.925 65	0.923 41
0.670 74	0.962 81	0.959 49	0.957 27	0.953 95	0.951 75	0.948 39	0.946 15	0.942 80	0.940 51	0.937 07	0.934 79
0.694 67	0.969 24	0.965 90	0.963 67	0.960 33	0.958 10	0.954 73	0.952 50	0.949 12	0.946 82	0.943 36	0.941 08
0.751 12	0.984 82	0.981 41	0.979 15	0.975 75	0.973 48	0.970 07	0.967 78	0.964 36	0.962 02	0.958 51	0.956 18
0.800 60	0.999 03	0.995 58	0.993 28	0.989 85	0.987 55	0.984 08	0.981 79	0.978 33	0.975 96	0.972 40	0.970 06
0.901 90	1.030 04	1.026 50	1.024 14	1.020 62	1.018 27	1.014 71	1.012 37	1.008 81	1.006 40	1.002 75	1.000 36
0.951 68	1.046 17	1.042 59	1.040 21	1.036 65	1.034 28	1.030 70	1.028 33	1.024 73	1.022 30	1.018 62	1.016 20

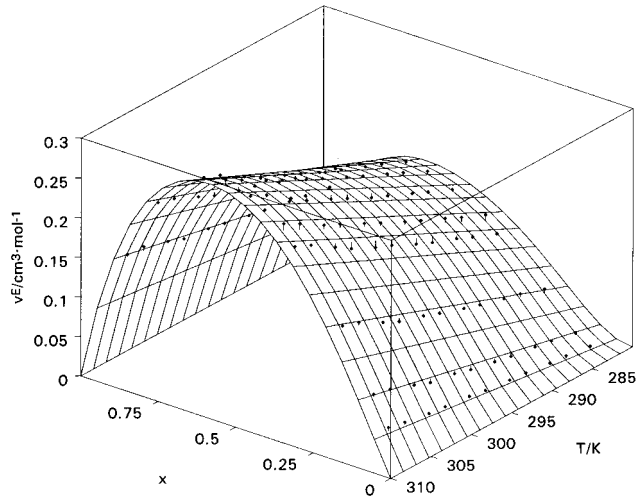

Figure 1. Excess molar volumes v^E for the system nitroethane + 1-butanol in the temperature interval (283.15−308.15) K over the whole composition range: (●) experimental points. (Grid lines) eq 6.

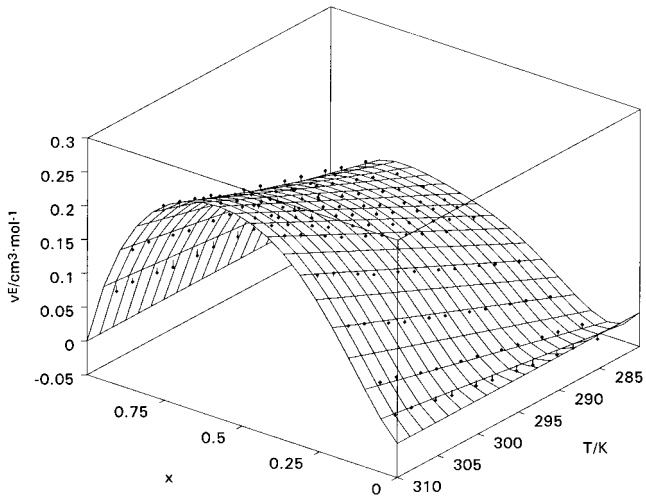

Figure 2. Excess molar volumes v^E for the system nitroethane + 2-methyl-1-propanol in the temperature interval (283.15−308.15) K over the whole composition range: (●) experimental points; (grid lines) eq 6.

molecular weight, and subscripts denote properties of the pure products. The volume fraction of component 1 ϕ is defined by

$$\phi = \frac{\rho}{\rho_1} xM_1/(xM_1 + (1 - x)M_2) \qquad (5)$$

Table 4. Speeds of Sound, u, for the Mixtures in the Temperature Range (283.15−308.15) K

	u/m·s^{-1}										
x	283.15 K	286.15 K	288.15 K	291.15 K	293.15 K	296.15 K	298.15 K	301.15 K	303.15 K	306.15 K	308.15 K
						x Nitroethane + (1 − x) 1-Butanol					
0.055 30	1291.30	1280.82	1273.81	1263.28	1256.37	1246.01	1239.11	1228.81	1221.91	1211.74	1205.13
0.103 38	1290.78	1280.37	1273.40	1262.80	1255.79	1245.38	1238.41	1228.03	1221.14	1210.89	1204.36
0.204 27	1290.59	1280.09	1273.02	1262.26	1255.21	1244.63	1237.54	1227.06	1220.10	1209.67	1203.10
0.358 52	1291.10	1280.49	1273.27	1262.44	1255.22	1244.46	1237.35	1226.59	1219.53	1208.94	1202.35
0.394 95	1291.95	1281.06	1273.80	1262.79	1255.67	1244.85	1237.69	1226.89	1219.75	1209.04	1202.17
0.502 34	1293.25	1282.51	1275.33	1264.32	1257.11	1246.22	1238.97	1228.19	1221.00	1210.29	1203.63
0.582 56	1297.00	1285.96	1278.60	1267.51	1260.22	1249.29	1242.00	1231.08	1223.78	1212.97	1205.96
0.652 34	1299.30	1288.42	1281.15	1269.98	1262.65	1251.64	1244.31	1233.35	1226.14	1215.22	1208.42
0.800 40	1310.68	1299.65	1292.23	1280.86	1273.41	1262.15	1254.69	1243.53	1236.15	1225.07	1218.13
0.897 94	1322.59	1311.30	1303.70	1292.06	1284.37	1272.89	1265.22	1253.78	1246.14	1234.77	1227.73
						x Nitroethane + (1 − x) 2-Methyl-1-propanol					
0.055 13	1242.51	1232.24	1225.36	1214.82	1207.93	1197.62	1190.75	1180.46	1173.70	1163.53	1157.12
0.103 94	1245.19	1234.83	1227.85	1217.23	1210.32	1199.85	1192.91	1182.61	1175.76	1165.55	1159.09
0.207 66	1250.79	1240.29	1233.23	1222.53	1215.46	1204.90	1197.85	1187.34	1180.36	1169.92	1163.33
0.307 31	1256.08	1245.57	1238.44	1227.71	1220.61	1209.97	1202.82	1192.19	1185.17	1174.63	1167.95
0.455 16	1265.46	1254.90	1247.79	1236.93	1229.79	1219.05	1211.88	1201.18	1194.01	1183.37	1176.66
0.508 06	1275.79	1260.95	1252.52	1241.01	1233.82	1223.03	1215.84	1205.08	1197.94	1187.24	1180.57
0.549 55	1272.99	1262.37	1255.20	1244.29	1237.04	1226.22	1218.98	1208.20	1201.00	1190.26	1183.46
0.618 64	1280.03	1269.33	1262.15	1251.09	1243.84	1232.89	1225.65	1214.78	1207.58	1196.76	1189.92
0.702 29	1289.31	1278.40	1271.08	1259.93	1252.62	1241.57	1234.21	1223.18	1215.92	1204.96	1198.02
0.803 99	1303.32	1292.27	1284.80	1273.43	1265.94	1254.68	1247.22	1235.97	1228.58	1217.42	1210.41
0.902 79	1320.18	1308.77	1301.17	1289.46	1281.74	1270.24	1262.50	1251.01	1243.36	1231.91	1224.75
0.954 20	1329.68	1317.98	1310.15	1298.11	1290.26	1278.41	1270.53	1258.75	1250.97	1239.26	1231.94
						x Nitroethane + (1 − x) 2-Butanol					
0.059 89	1266.02	1255.24	1247.97	1236.83	1229.52	1218.48	1211.13	1200.08	1192.73	1181.72	1174.80
0.097 71	1266.58	1255.72	1248.32	1237.22	1229.80	1218.73	1211.31	1200.17	1192.82	1181.76	1174.82
0.206 01	1268.32	1257.33	1249.93	1238.67	1231.24	1220.10	1212.61	1201.43	1194.03	1182.87	1175.89
0.309 19	1270.94	1259.96	1252.56	1241.23	1233.76	1222.53	1215.04	1203.84	1196.37	1185.18	1178.06
0.352 70	1272.32	1261.36	1253.98	1242.62	1235.18	1223.94	1216.42	1205.21	1197.73	1186.56	1179.55
0.404 90	1274.43	1263.48	1256.10	1244.76	1237.31	1226.05	1218.57	1207.32	1199.94	1188.78	1181.71
0.496 74	1279.62	1268.57	1261.13	1249.78	1242.30	1231.04	1223.50	1212.21	1204.77	1193.60	1186.64
0.515 21	1280.71	1269.71	1262.29	1250.91	1243.40	1232.15	1224.67	1213.45	1206.02	1194.86	1187.95
0.517 54	1280.85	1269.88	1262.41	1251.02	1243.57	1232.23	1224.72	1213.45	1205.98	1194.79	1187.63
0.615 30	1287.80	1276.75	1269.24	1257.86	1250.31	1238.99	1231.42	1220.13	1212.65	1201.45	1194.37
0.625 69	1288.73	1277.62	1270.15	1258.73	1251.17	1239.89	1232.33	1221.11	1213.64	1202.43	1195.36
0.670 74	1292.52	1281.40	1273.90	1262.41	1254.87	1243.51	1235.91	1224.60	1217.09	1205.83	1198.69
0.694 67	1295.08	1283.73	1276.18	1264.73	1257.13	1245.76	1238.18	1226.88	1219.35	1208.15	1200.98
0.751 12	1300.77	1289.51	1281.96	1270.43	1262.85	1251.40	1243.75	1232.41	1224.80	1213.50	1206.35
0.800 60	1306.81	1295.57	1287.91	1276.34	1268.69	1257.19	1249.54	1238.13	1230.51	1219.18	1211.96
0.901 90	1321.59	1310.00	1302.36	1290.56	1282.69	1270.92	1263.13	1251.44	1243.71	1232.10	1224.83
0.951 68	1329.28	1317.68	1309.79	1297.77	1289.85	1277.96	1270.08	1258.25	1250.43	1238.76	1231.35

The excess molar volumes have been fitted simultaneously against temperature and composition to Redlich−Kister polynomials according to the expression

$$v^{E}/\mathrm{cm}^3\cdot\mathrm{mol}^{-1} = x(1-x)\sum_{i=1}^{5}\sum_{j=1}^{3} A_{ij}10^{1-j}(2x-1)^{i-1}(T/\mathrm{K}-T_0)^{j-1} \quad (6)$$

Again, Marquardt's algorithm was used in the fitting process. The coefficients A_{ij} are given in Table 7.

Figures 1−3 are 3-D representations of the excess molar volumes for each system. The excess molar volumes are positive in both temperature and composition ranges covered for both nitroethane + 1-butanol and nitroethane + 2-butanol. Nevertheless, the excess molar volumes of the nitroethane + 2-methyl-1-propanol system are negative at small composition of nitroethane and at low temperatures. The system containing 2-butanol has higher excess molar volumes than the other ones. Increasing temperature, the excess molar volumes increase for all systems as shown in Figure 4, where equimolar values are given. Also, the mixture containing 2-butanol appears to be more sensitive to temperature changes. Excess isobaric thermal expansivities at 298.15 K are represented in Figure 5; positive values are obtained in all cases that are higher for nitroethane + 2-butanol.

Table 5. Coefficients A_{ij}/g·cm^{-3}·K^{1-j} of Eq 2 and Standard Deviations, s

	i				
j	1	2	3	4	5
	x Nitroethane + (1 − x) 1-Butanol (s = 0.000 07 g·cm^{-3})				
1	0.819 366	0.189 230	0.044 819	−0.003 003	0.015 855
2	−0.007 561	−0.004 228	−0.000 548	0.000 123	0.000 308
3	−0.000 027	−0.000 341	0.000 958	−0.001 143	0.000 488
	x Nitroethane + (1 − x) 2-Methyl-1-propanol (s = 0.000 10 g·cm^{-3})				
1	0.811 60	0.196 60	0.042 14	0.000 27	0.015 55
2	−0.007 53	−0.005 30	0.002 07	−0.002 47	0.001 33
3	−0.000 07	−0.000 21	0.000 66	−0.000 75	0.000 29
	x Nitroethane + (1 − x) 2-Butanol (s = 0.000 07 g·cm^{-3})				
1	0.816 890	0.181 120	0.069 444	−0.033 675	0.032 468
2	−0.007 680	−0.007 553	0.007 981	−0.007 777	0.003 149
3	−0.000 183	0.000 391	−0.000 897	0.001 009	−0.000 391

The temperature and composition dependence of the excess molar volumes of mixtures containing 1-alcohol + alkane is explained by some authors (Treszczanowicz et al.;[11] Ott et al.[12]) as a balance between positive contributions (mainly due to hydrogen bond rupture and dispersive interactions between unlike molecules) and negative contributions (due to packing effects). For alcohol + polar mixtures these contributions also take place. Bittrich and Eckert[13] showed the evidence of complex formations

Table 6. Coefficients A_{ij}/m·s^{-1}·K^{1-j} of Eq 2 and Standard Deviations, s

		i						
j	1	2	3	4	5	6	7	8
	x Nitroethane + (1 − x) 1-Butanol (s = 0.2 m·s^{-1})							
1	1300.3	26.2	−223.4	677.2	−536.3	−704.6	1484.57	−676.14
2	−34.0	−13.1	77.7	−323.5	714.6	−831.14	482.4	−112.3
	x Nitroethane + (1 − x) 2-Methyl-1-Propanol (s = 0.2 m·s^{-1})							
3	1247.5	97.4	−184.1	−126.5	2306.3	−5136.4	4773.2	−1629.4
1	−33.6	−13.5	30.8	41.4	−359.0	704.3	−600.7	190.6
	x Nitroethane + (1 − x) 2-Butanol (s = 0.1 m·s^{-1})							
3	1274.9	46.8	−218.3	500.1	325.2	−2182.9	2587.6	−985.4
	−35.8	−18.9	101.8	−277.8	385.2	−233.0	5.8	33.0

Table 7. Coefficients A_{ij} and Standard Deviations for the Fits of the Isentropic Compressibilities, κ_S, and for Excess Molar Volumes, v^E

		i				
magnitude	j	1	2	3	4	5
	x Nitroethane + (1 − x) 1-Butanol A_{ij}/TPa^{-1}·K^{1-j} (s = 0.3 TPa^{-1})					
κ_S	1	721.10	−180.50	79.34	−151.10	46.88
	2	45.30	−5.54	9.83	−32.63	19.46
	3	1.83	2.14	−5.44	5.75	−2.35
	A_{ij}/cm^3·mol·K^{1-j} (s = 0.003 cm^3·mol^{-1})					
v^E	1	0.5601	0.3393	0.1357	0.2892	−0.0305
	2	0.1679	0.0116	−0.0932	0.0413	0.1790
	3	0.0127	−0.0048	0.0329	−0.0169	−0.0363
	x Nitroethane + (1 − x) 2-Methyl-1-Propanol Aij/TPa^{-1}·K^{1-j} (s = 0.4 TPa^{-1})					
κ_S	1	791.00	−304.50	241.00	−367.50	155.50
	2	50.83	−5.01	−29.54	29.46	−9.30
	3	2.25	1.17	−1.46	−1.12	1.09
	Aij/cm^3·mol·K^{1-j} (s = 0.004 cm^3·mol)					
v^E	1	0.3281	0.3337	0.1705	0.6525	−0.3204
	2	0.2049	−0.0070	0.0086	−0.0390	0.0885
	3	0.0101	−0.0065	0.0203	−0.0039	−0.0313
	x Nitroethane + (1 − x) 2-Butanol Aij/TPa^{-1}·K^{1-j} (s = 0.3 TPa^{-1})					
κ_S	1	751.80	−188.80	16.30	−110.40	46.83
	2	49.15	2.61	−37.73	33.18	−10.80
	3	2.99	−0.01	−2.38	2.28	−0.99
	Aij/cm^3·mol·K^{1-j} (s = 0.003 cm^3·mol)					
v^E	1	1.1030	0.2433	0.7297	0.4465	−0.5963
	2	0.3005	−0.0556	0.0597	−0.1487	0.0679
	3	−0.0002	0.0017	−0.0029	0.0065	−0.0024

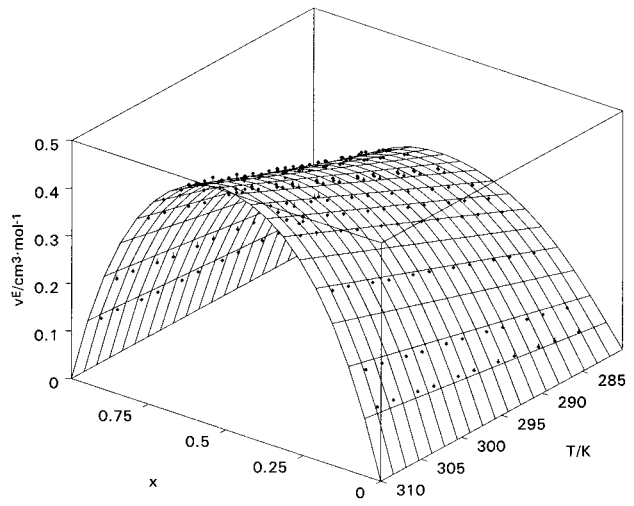

Figure 3. Excess molar volumes v^E for the system nitroethane + 2-butanol in the temperature interval (283.15−308.15) K over the whole composition range: (●) experimental points; (grid lines) eq 6.

between unlike molecules for alcohol + nitroalkane mixtures in the framework of an association model; this results in a negative contribution to v^E.

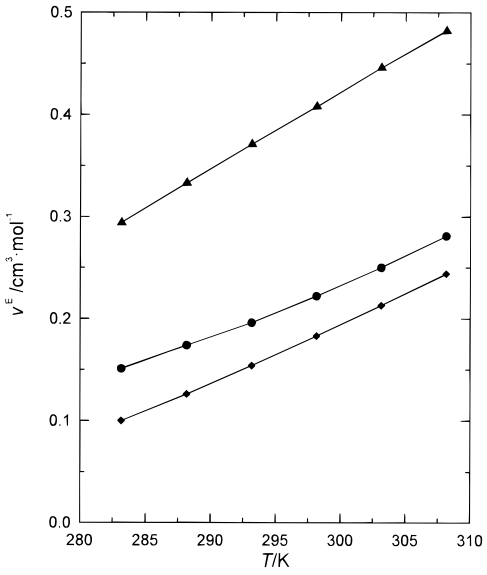

Figure 4. Excess molar volumes v^E at equimolar composition (x = 0.5): (●) x nitroethane + (1 − x) 1-butanol; (◆) x nitroethane + (1 − x) 2-methyl-1-propanol; (▲) x nitroethane + (1 − x) 2-butanol.

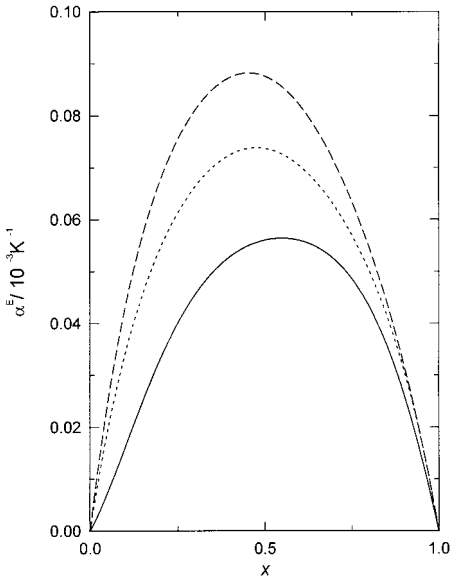

Figure 5. Excess isobaric thermal expansivities α^E at 298.15 K: (—) x nitroethane + (1 − x) 1-butanol; (- - -) x nitroethane + (1 − x) 2-methyl-1-propanol; (— — —) x nitroethane + (1 − x) 2-butanol.

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