

Temperature Dependence of Thermophysical Properties of Hexane + 1-Hexanol

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The aim of this work is to complete our studies on physical properties of binary mixtures of alkane + 1-alkanols. This work reports densities, refractive indices, speeds of sound, and isentropic compressibilities of the mixture of hexane with 1-hexanol at different temperatures, from 288.15 K to 308.15 K. From the experimental values, the corresponding excess and deviation values were computed (excess molar volumes, changes of refractive index upon mixing, changes of speed of sound upon mixing, and changes of isentropic compressibilities upon mixing). Variable-degree polynomials were fitted to the results. A comparative study of these results with other available physical properties of the same mixture was performed. Excess molar volumes were compared with the predictions of the Nitta–Chao Group contribution model.

Introduction

Continuing a series of theoretical and experimental works^{1–11} on binary mixtures alkane + 1-alkanol, refractive indices, speed of sound, and isentropic compressibilities of the binary mixtures of hexane and octane with (1-butanol, 1-hexanol, and 1-octanol), at 298.15 K and atmospheric pressure, were published.^{12,13} Recently, a study of these properties with temperature was performed.¹⁴ As a continuation, this paper reports densities (ρ), refractive indices (n_D), and speeds of sound (u) and the corresponding derived values of hexane with 1-hexanol, which were measured at the temperatures of 288.15 K, 293.15 K, 303.15 K, and 308.15 K and atmospheric pressure, over the entire range of composition. Excess molar volume values of this mixture were found in the literature¹⁵ at 288.15 K, 298.15 K, 308.15 K, and 323.15 K and speeds of sound^{16,17} at 298.15 K and 303.15 K.

Experimental Section

The hexane employed was supplied by Fluka and the 1-hexanol by Merck. Their mole fraction purities were as follows: hexane (>0.995) and 1-hexanol (>0.98). These values were checked by a gas–liquid chromatographic test, being in accordance with vendor specifications. The substances were degassed and dried over molecular sieves (Union Carbide, type 0.4 nm). Precautions such as cooling chemicals before sample preparation and minimizing empty space in vessels were taken to avoid evaporation losses during manipulations and then possible errors in calculations.

The refractive index was measured with an automatic refractometer, ABBEMAT-HP Dr. Kernchen, with a precision of $\pm 10^{-5}$. To keep a constant temperature, the measuring prism was thermostated using a PolyScience controller bath model 9510 with a temperature stability

Table 1. Comparison of the Density, ρ , Refractive Index, n_D , and Speed of Sound, u , of the Pure Liquids with the Available Literature Data at Different Temperatures

compound	T (K)	ρ (g·cm ⁻³)		n_D		u (m·s ⁻¹)	
		expt.	lit.	expt.	lit.	expt.	lit.
hexane	288.15	0.6642	0.6640 ^a	1.37774		1122	
	293.15	0.6597	0.65940 ^b	1.37516	1.37486 ^c	1100	1099.8 ^b
	298.15	0.6552	0.65520 ^d	1.37207	1.3720 ^c	1077	1076.3 ^e
	303.15	0.6506	0.65063 ^f	1.36947	1.3695 ^c	1055	1054.6 ^g
	308.15	0.6460	0.64586 ^h	1.36626	1.3662 ⁱ	1032	1032.4 ^g
1-hexanol	288.15	0.8223	0.82214 ^b	1.41966		1337	
	293.15	0.8187	0.81890 ^f	1.41798	1.4181 ^c	1323	
	298.15	0.8151	0.81507 ^d	1.41595	1.4157 ^c	1303	1302.45 ^k
	303.15	0.8118	0.81195 ^d	1.41428	1.4137 ^m	1287	1287 ^l
	308.15	0.8081	0.80793 ^b	1.41182	1.4114 ^m	1270	

^a Reference 18. ^b Reference 19. ^c Reference 20. ^d Reference 1. ^e Reference 21. ^f Reference 22. ^g Reference 23. ^h Reference 15. ⁱ Reference 24. ^j Reference 25. ^k Reference 26. ^l Reference 27. ^m Reference 28.

of $\pm 10^{-2}$ K. Triply distilled water and air were used for refractometer calibration.

The density and speed of sound of the mixtures and pure liquids were measured with an Anton Paar DSA-48 densimeter and sound analyzer with a precision of $\pm 5 \times 10^{-5}$ g·cm⁻³ and $\pm 10^{-1}$ m·s⁻¹, respectively. The density measuring cell is thermostated with a temperature stability of $\pm 10^{-2}$ K. The apparatus calibration was performed periodically. Triply distilled water was used for calibrating the speed of sound cell.

The experimental techniques and operation mode have been described previously.¹² The samples were prepared by mass using a Mettler AE-240 balance with a precision of $\pm 1 \times 10^{-4}$ in mole fraction, covering the whole composition range of the mixture.

Results and Discussion

Densities, refractive indices, and speeds of sound at different temperatures, of the pure component liquid are listed in Table 1, together with literature values. The

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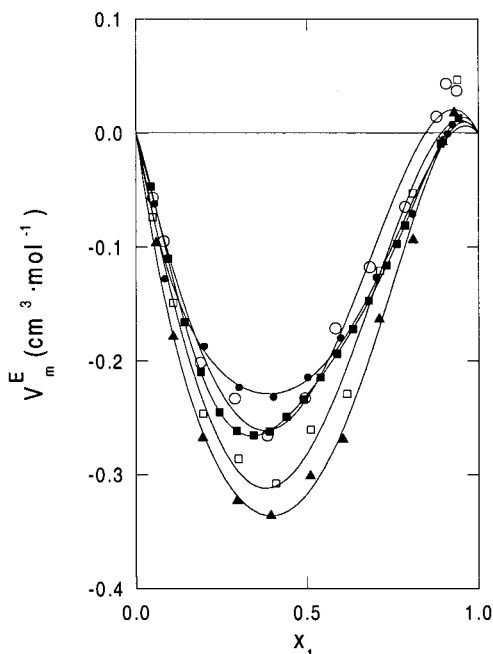


Figure 1. Excess molar volume for hexane (1) + 1-hexanol (2): (●) 288.15 K; (○) 293.15 K; (■) 298.15 K; (□) 303.15 K; (▲) 308.15 K; (---) eq 3.

Table 2. Refractive Indices, n_D , and Changes of Refractive Indices upon Mixing, Δn_D , for Hexane (1) + 1-Hexanol (2) at Different Temperatures

x_1	n_D	Δn_D	x	n_D	Δn_D
T = 288.15 K					
0.0000	1.41966		0.0000	1.41798	
0.0501	1.41817	0.00061	0.0501	1.41599	0.00016
0.0902	1.41677	0.00089	0.0902	1.41455	0.00043
0.1911	1.41306	0.00141	0.1911	1.41060	0.00080
0.2899	1.40906	0.00155	0.2899	1.40650	0.00093
0.3830	1.40507	0.00147	0.3830	1.40260	0.00102
0.4898	1.40015	0.00102	0.4898	1.39792	0.00091
0.5851	1.39591	0.00078	0.5851	1.39355	0.00062
0.6906	1.39113	0.00042	0.6906	1.38880	0.00039
0.7823	1.38710	0.00023	0.7823	1.38455	0.00007
0.8781	1.38282	-0.00003	0.8781	1.38025	-0.00013
0.9277	1.38073	-0.00004	0.9277	1.37812	-0.00014
1.0000	1.37774		1.0000	1.37516	
T = 293.15 K					
0.0000	1.41428		0.0000	1.41182	
0.0605	1.41180	0.00023	0.0605	1.40943	0.00037
0.0909	1.41060	0.00039	0.0909	1.40815	0.00047
0.1995	1.40596	0.00062	0.1995	1.40368	0.00095
0.3581	1.39915	0.00092	0.3581	1.39670	0.00120
0.3902	1.39773	0.00093	0.3902	1.39526	0.00122
0.4902	1.39310	0.00079	0.4902	1.39086	0.00137
0.5811	1.38870	0.00046	0.5811	1.38662	0.00127
0.6886	1.38350	0.00008	0.6886	1.38134	0.00089
0.7960	1.37850	-0.00011	0.7960	1.37558	0.00003
0.8925	1.37400	-0.00029	0.8925	1.37148	0.00032
0.9261	1.37250	-0.00028	0.9261	1.36925	-0.00038
1.0000	1.36947		1.0000	1.36626	
T = 303.15 K					
0.0000	1.41428		0.0000	1.41182	
0.0605	1.41180	0.00023	0.0605	1.40943	0.00037
0.0909	1.41060	0.00039	0.0909	1.40815	0.00047
0.1995	1.40596	0.00062	0.1995	1.40368	0.00095
0.3581	1.39915	0.00092	0.3581	1.39670	0.00120
0.3902	1.39773	0.00093	0.3902	1.39526	0.00122
0.4902	1.39310	0.00079	0.4902	1.39086	0.00137
0.5811	1.38870	0.00046	0.5811	1.38662	0.00127
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0.8925	1.37400	-0.00029	0.8925	1.37148	0.00032
0.9261	1.37250	-0.00028	0.9261	1.36925	-0.00038
1.0000	1.36947		1.0000	1.36626	
T = 308.15 K					
0.0000	1.41428		0.0000	1.41182	
0.0605	1.41180	0.00023	0.0605	1.40943	0.00037
0.0909	1.41060	0.00039	0.0909	1.40815	0.00047
0.1995	1.40596	0.00062	0.1995	1.40368	0.00095
0.3581	1.39915	0.00092	0.3581	1.39670	0.00120
0.3902	1.39773	0.00093	0.3902	1.39526	0.00122
0.4902	1.39310	0.00079	0.4902	1.39086	0.00137
0.5811	1.38870	0.00046	0.5811	1.38662	0.00127
0.6886	1.38350	0.00008	0.6886	1.38134	0.00089
0.7960	1.37850	-0.00011	0.7960	1.37558	0.00003
0.8925	1.37400	-0.00029	0.8925	1.37148	0.00032
0.9261	1.37250	-0.00028	0.9261	1.36925	-0.00038
1.0000	1.36947		1.0000	1.36626	

experimental results of the refractive index, n_D , at all studied temperatures are reported in Table 2.

The experimental results of density, ρ , speed of sound, u , and calculated isentropic compressibility, κ_S ($\kappa_S = \rho^{-1}u^{-2}$), are reported in Table 3.

The values of excess molar volumes were computed using the following equation,

$$V_m^E = \sum_{i=1}^2 x_i M_i (\rho^{-1} - \rho_i^{-1}) \quad (1)$$

where x is the mole fraction, M the molecular weight, and

Table 3. Densities, ρ , Speeds of Sound, u , Isentropic Compressibilities, κ_S , Excess Molar Volumes, V^E , Changes of Speeds of Sound upon Mixing, Δu , and Changes of Isentropic Compressibilities upon Mixing, $\Delta\kappa_S$, for Hexane (1) + 1-Hexanol (2) at Different Temperatures

x_1	ρ g·cm ⁻³	u m·s ⁻¹	κ_S TPa ⁻¹	V^E cm ³ ·mol ⁻¹	Δu m·s ⁻¹	$\Delta\kappa_S$ TPa ⁻¹
T = 288.15 K						
0.0000	0.8223	1337.0	680.3			
0.0547	0.8137	1322.3	702.9	-0.063	-2.9	-5.6
0.0847	0.8092	1314.9	714.7	-0.128	-3.8	-9.3
0.1991	0.7909	1283.6	767.4	-0.187	-10.6	-15.5
0.3006	0.7747	1256.9	817.1	-0.223	-15.6	-18.1
0.4019	0.7585	1231.2	869.8	-0.232	-19.9	-17.6
0.5025	0.7424	1207.1	924.4	-0.214	-21.9	-14.9
0.5983	0.7271	1187.1	976.0	-0.180	-21.4	-12.6
0.7020	0.7106	1165.5	1035.9	-0.127	-20.7	-6.1
0.8073	0.6940	1147.1	1095.1	-0.071	-16.5	-1.1
0.9099	0.6779	1131.5	1152.1	-0.001	-10.0	3.0
0.9247	0.6756	1129.5	1160.3	0.007	-8.9	3.5
1.0000	0.6642	1122.2	1195.5			
T = 293.15 K						
0.0000	0.8187	1322.6	698.3			
0.0492	0.8109	1306.5	722.5	-0.057	-5.2	-3.1
0.0815	0.8058	1297.5	737.1	-0.095	-6.9	-6.4
0.1889	0.7888	1268.2	788.2	-0.202	-12.3	-14.8
0.2888	0.7727	1241.3	839.9	-0.233	-17.0	-18.4
0.3834	0.7576	1216.6	891.7	-0.266	-20.6	-19.1
0.4933	0.7398	1189.5	955.4	-0.233	-23.4	-16.3
0.5831	0.7252	1168.6	1009.7	-0.171	-24.2	-11.8
0.6836	0.7091	1147.7	1070.6	-0.118	-22.8	-6.5
0.7858	0.6929	1128.7	1132.9	-0.065	-19.1	-0.9
0.8784	0.6782	1113.4	1189.4	0.014	-13.7	4.3
0.9061	0.6738	1109.3	1206.1	0.043	-11.7	5.6
0.9377	0.6690	1105.3	1223.6	0.037	-8.7	5.6
1.0000	0.6597	1100.1	1252.5			
T = 303.15 K						
0.0000	0.8118	1286.7	744.0			
0.0477	0.8042	1272.9	767.4	-0.074	-2.7	-7.0
0.1075	0.7946	1255.5	798.3	-0.149	-6.3	-14.2
0.1948	0.7806	1230.7	845.8	-0.246	-10.9	-22.4
0.2982	0.7637	1201.3	907.3	-0.286	-16.3	-26.8
0.4069	0.7460	1171.7	976.3	-0.308	-20.6	-27.1
0.5094	0.7291	1145.3	1045.7	-0.261	-23.3	-23.1
0.6155	0.7119	1120.3	1119.1	-0.229	-23.6	-17.3
0.7120	0.6960	1099.5	1188.6	-0.121	-22.1	-9.4
0.8078	0.6806	1081.3	1256.7	-0.053	-18.1	-2.3
0.8963	0.6666	1066.5	1318.8	-0.007	-12.3	3.4
0.9386	0.6598	1060.1	1348.5	0.047	-8.9	6.1
1.0000	0.6506	1054.8	1381.5			
T = 308.15 K						
0.0000	0.8081	1269.7	767.6			
0.0587	0.7987	1252.8	797.7	-0.096	-2.9	-10.2
0.1077	0.7909	1238.5	824.3	-0.179	-5.6	-17.2
0.1934	0.7770	1213.2	874.4	-0.268	-10.5	-25.8
0.2948	0.7604	1183.8	938.3	-0.323	-15.8	-31.4
0.3933	0.7442	1156.2	1005.1	-0.336	-19.9	-32.2
0.5084	0.7252	1126.1	1087.5	-0.301	-22.8	-28.7
0.6033	0.7097	1103.3	1157.6	-0.269	-23.0	-23.7
0.7100	0.6921	1079.3	1240.2	-0.163	-21.6	-14.1
0.8085	0.6762	1060.1	1315.9	-0.094	-17.5	-6.0
0.8941	0.6624	1045.3	1381.7	-0.008	-11.9	1.1
0.9294	0.6568	1039.8	1408.3	0.018	-9.1	3.5
1.0000	0.6460	1032.1	1453.2			

the corresponding quantities with subscript i referring to pure chemicals.

Changes of refractive index upon mixing Δn_D , changes of speed of sound upon mixing Δu , and changes of isentropic compressibility upon mixing $\Delta\kappa_S$ were evaluated for each composition point using the following equation:

$$\Delta Q = Q - \sum_{i=1}^2 x_i Q_i \quad (2)$$

In these equations, $Q = n_D$, u , or κ_S and ΔQ is the change upon mixing property (Δn_D , Δu , or $\Delta\kappa_S$). The excess molar

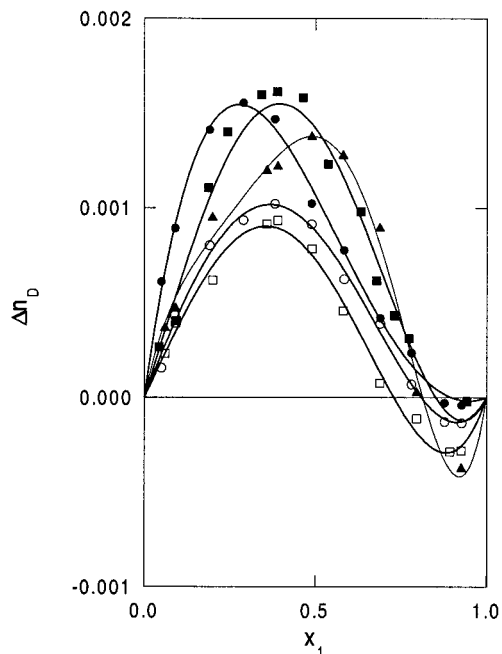


Figure 2. Changes of refractive index upon mixing for hexane (1) + 1-hexanol (2): (●) 288.15 K; (○) 293.15 K; (■) 298.15 K; (□) 303.15 K; (▲) 308.15 K; (—) eq 3.

Table 4. Parameters A_p in Equation 3 and Standard Deviations σ for Hexane (1) + 1-Hexanol (2)

	A_0	A_1	A_2	A_3	A_4	σ
$T = 288.15$ K						
V_m^E (cm ³ ·mol ⁻¹)	-0.866	0.449	0.179	0.591		0.001
Δn_D	0.0043	-0.0069	0.0019			0.0001
Δu (m·s ⁻¹)	-85.8	-24.2	-29.3	-26.1		0.5
$\Delta \kappa_S$ (TPa ⁻¹)	-62.9	58.0	34.0	50.5		0.6
$T = 293.15$ K						
V_m^E (cm ³ ·mol ⁻¹)	-0.927	0.756	0.615	0.379		0.001
Δn_D	0.0035	-0.0039	-0.0028			0.0001
Δu (m·s ⁻¹)	-94.7	-30.2	14.4	3.94	-67.6	0.2
$\Delta \kappa_S$ (TPa ⁻¹)	-62.5	73.7	1.17	25.8	116.9	0.4
$T = 298.15$ K						
V_m^E (cm ³ ·mol ⁻¹)	-0.9180	0.7422	-0.3797	0.0863	1.1854	0.002
Δn_D	0.0057	-0.0047	-0.0045			0.002
Δu (m·s ⁻¹)	-88.1	-29.6	3.3	-16.6	23.2	0.3
$\Delta \kappa_S$ (TPa ⁻¹)	-86.8	75.2	50.9	43.0		0.7
$T = 303.15$ K						
V_m^E (cm ³ ·mol ⁻¹)	-1.12	0.976	0.589			0.016
Δn_D	0.0029	-0.0046	-0.0038			0.0001
Δu (m·s ⁻¹)	-92.5	-32.3	11.6	-19.7	-36.2	0.2
$\Delta \kappa_S$ (TPa ⁻¹)	-94.3	85.8	9.14	59.2	93.3	0.7
$T = 308.15$ K						
V_m^E (cm ³ ·mol ⁻¹)	-1.27	0.743	0.459	0.578		0.010
Δn_D	0.0055	-0.0004	-0.0072	-0.0097		0.0001
Δu (m·s ⁻¹)	-90.7	-29.5	7.73	-23.4	-18.5	0.1
$\Delta \kappa_S$ (TPa ⁻¹)	-116.6	83.7	15.6	62.5	66.3	0.5

^a Reference 12.

volumes and change upon mixing properties values are given in Tables 2 and 3.

Uncertainty in the changes upon mixing was estimated to be better than $\pm 2 \times 10^{-5}$ for the refractive index, ± 1.1 m·s⁻¹ for the speed of sound, and ± 2.7 TPa⁻¹ for the isentropic compressibilities and $\pm 2 \times 10^{-2}$ cm³·mol⁻¹ for excess molar volume.

The values were correlated by means of the Redlich-Kister expression²⁹ for every binary mixture,

$$\Delta Q = x(1-x) \sum_{p=0}^M A_p (2x-1)^p \quad (3)$$

where x is the molar fraction of hexane, A_p stands for the

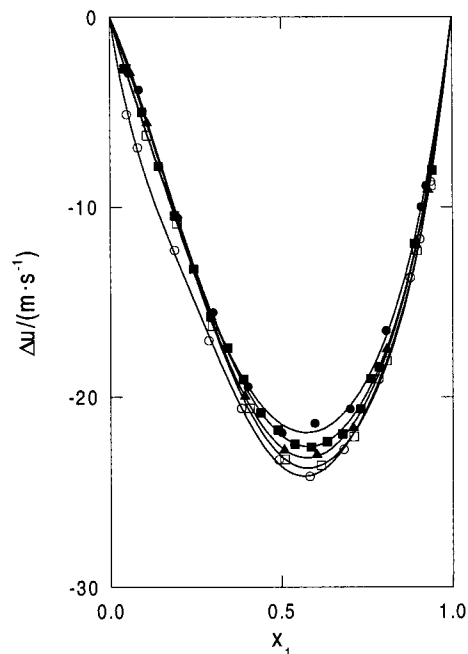


Figure 3. Changes of speed of sound upon mixing for hexane (1) + 1-hexanol (2): (●) 288.15 K; (○) 293.15 K; (■) 298.15 K; (□) 303.15 K; (▲) 308.15 K; (—) eq 3.

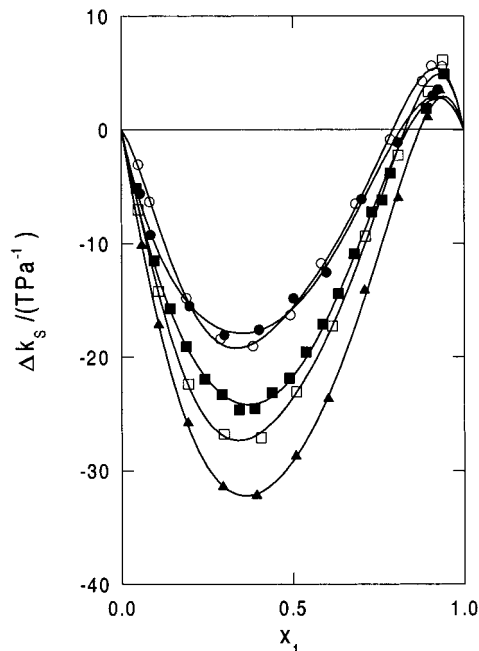


Figure 4. Changes of isentropic compressibilities upon mixing for hexane (1) + 1-hexanol (2): (●) 288.15 K; (○) 293.15 K; (■) 298.15 K; (□) 303.15 K; (▲) 308.15 K; (—) eq 3.

fitting parameters, and M is the degree of the polynomial expansion. An unweighted least-squares method was used to fit the data. The degree of the polynomials was optimized by applying the F-test.³⁰ These parameters are compiled in Table 4 as well as the root-mean-square deviations calculated according to the expression:

$$\sigma = \left(\sum_i^N \frac{(z_{\text{exp}} - z_{\text{cal}})^2}{N-n} \right)^{1/2} \quad (4)$$

where z_{exp} is the experimental value, z_{cal} is the calculated value, N is the number of experimental data points, and n

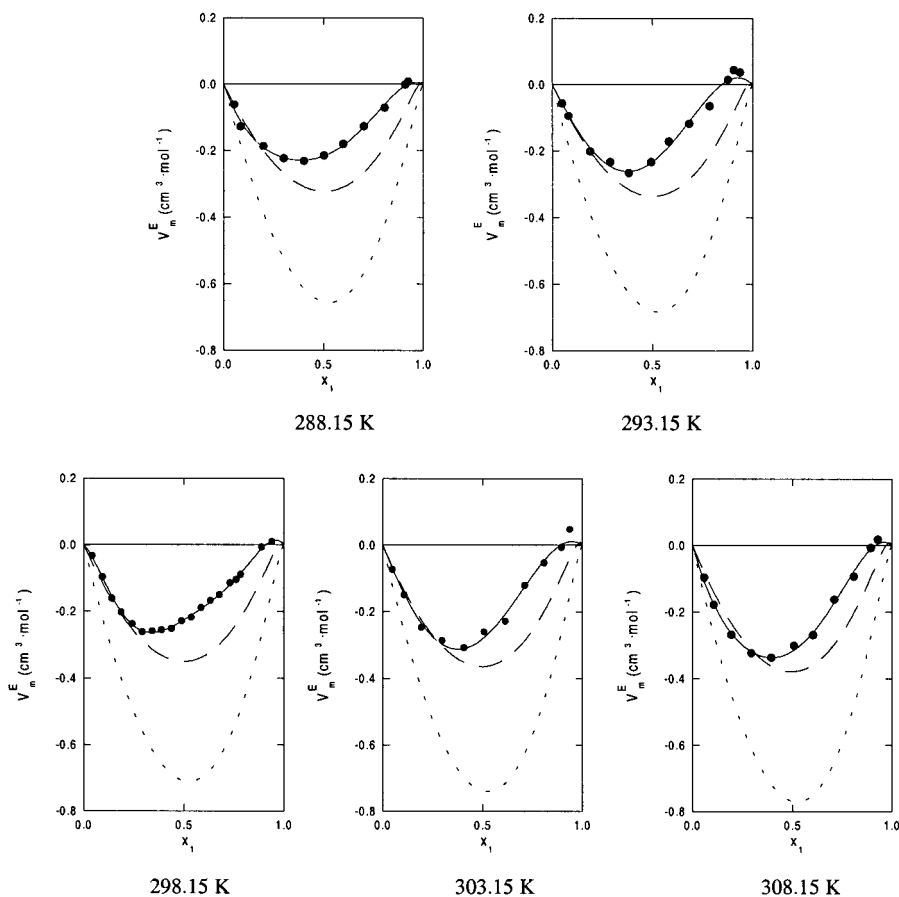


Figure 5. Excess molar volumes for hexane (1) + 1-hexanol (2) at 288.15 K, 293.15 K, 298.15 K, 303.15 K, and 308.15 K. (●) experimental values; (---) eq 3; (—) Nitta–Chao model with parameters of Fernández et al.;⁷ (- -) Nitta–Chao model with parameters of Nitta et al.³¹

is the number of fitting parameters A_p , used in eq 3.

Figure 1 shows excess molar volumes for hexane + 1-hexanol and the smoothed curves at the five temperatures. The values of V_m^E are negative for nearly the whole composition range at all temperatures, except for lower concentrations of 1-hexanol. This effect could be due to the disruption between alkanol self-association interactions. Changes of refractive index (Figure 2) show an opposite trend with V_m^E and do not present a systematic variation with temperature. Changes of speed of sound are negative, showing a minimum shifted toward higher hexane concentrations but variation with temperature is not regular (Figure 3). Changes of isentropic compressibilities upon mixing (Figure 4) present the same qualitative behavior as V_m^E curves, and both magnitudes become more negative when the temperature increases. Experimental values of excess molar volumes at 288.15 K, 298.15 K, and 308.15 K were compared at equimolar fraction with literature data, and average percent deviations were lower than 1.2% in all cases, except for 308.15 K, where this deviation value was 7%.

Excess molar volumes were compared in Figure 5 with the predictions of the Nitta–Chao group contribution model, using the old set of parameters obtained by Nitta et al.³¹ and the one recalculated by Fernández et al.⁷ As shown in this figure, the predictions with the parameters of Fernández et al. are better than those obtained using the old set of parameters. The Nitta–Chao model predictions of Fernández et al. present a positive region in the dilute region of 1-hexanol, in agreement with experimental curves, and describe this behavior.

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