Densities, Refractive Indices, Speeds of Sound, and Isentropic Compressibilities of Benzene + Cyclohexane + 1-Pentanol at 298.15 K

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Densities, refractive indices, speeds of sound, and isentropic compressibilities at 298.15 K for benzene + cyclohexane + 1-pentanol and the binary benzene + 1-pentanol and cyclohexane + 1-pentanol mixtures have been measured as a function of the mole fraction at atmospheric pressure. Densities and speeds of sound were determined by density and sound analyzer Anton Paar DSA-48 and refractive indices by the automatic refractometer ABBEMAT-HP Dr Kernchen.

Introduction

Separating azeotropic mixtures in pure components is a task commonly encountered in the chemical industry. The most important separation paths have in common the addition of a new component that alters the relative volatility, homogeneous azeotropic distillation being an economically attractive method. To study the capability

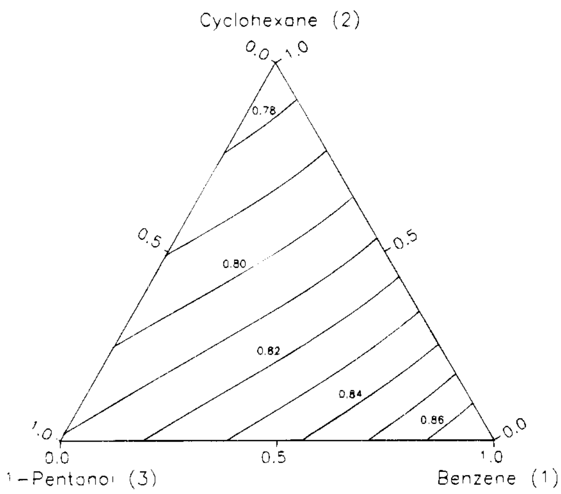

Figure 1. Density curves for benzene (1) + cyclohexane (2) + 1-pentanol (3) mixtures at 298.15 K.

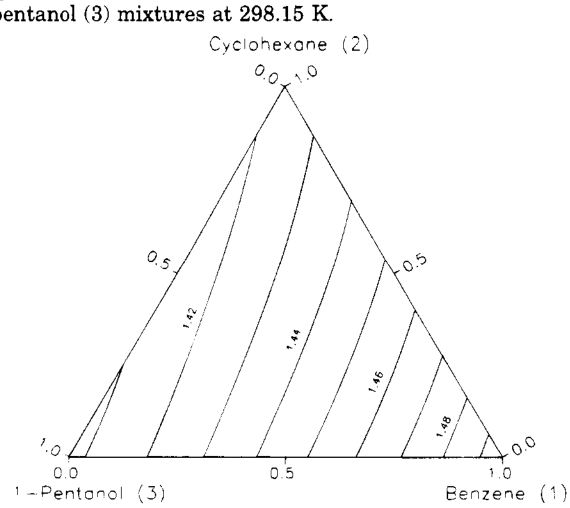

Figure 2. Refractive index curves for benzene (1) + cyclohexane (2) + 1-pentanol (3) mixtures at 298.15 K.

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Table 1. Comparison of Data with Literature Data for Pure Liquids at 298.15 K

	ϱ(298.15 K)/(g·cm^{-3})		n_D (298.15 K)		u(298.15 K)/(m·s^{-1})	
component	exptl	lit.	exptl	lit.	exptl	lit.
benzene	0.8736	0.87370 (*4*)	1.49692	1.49792 (*4*)	1299	1299.08 (*5*)
		0.87365 (*5*)		1.4967 (*6*)		1298.90 (*7*)
cyclohexane	0.7737	0.77389 (*4*)	1.42320	1.42354 (*4*)	1254	1253.78 (*5*)
		0.77385 (*5*)		1.4233 (*6*)		1253.28 (*7*)
1-pentanol	0.8110	0.8115 (*4*)	1.40787	1.4079 (*4*)	1276	1277 (*8*)
		0.8109 (*9*)		1.4079 (*10*)		

Table 2. Densities ϱ, Refractive Indices n_D, Speeds of Sound u, Isentropic Compressibilities κ_S, Excess Molar Volumes V_m^E, Changes of Refractive Index on Mixing δn_D, and Changes of Isentropic Compressibility on Mixing $\delta\kappa_S$ for Binary Mixtures at 298.15 K

x_1	ϱ/(g·cm^{-3})	n_D	u/(m·s^{-1})	κ_S/(TPa^{-1})	V_m^E/(cm^3·mol^{-1})	δn_D	$\delta\kappa_S$/(TPa^{-1})
Benzene (1) + 1-Pentanol (2)							
0.0000	0.8110	1.40782	1276	758	0.000	0.0000	0
0.0582	0.8136	1.41138	1273	758	0.057	−0.0016	5
0.1730	0.8191	1.41973	1269	758	0.140	−0.0035	14
0.2190	0.8214	1.42328	1267	758	0.170	−0.0041	18
0.3276	0.8270	1.43105	1264	756	0.237	−0.0060	25
0.3803	0.8298	1.43548	1263	755	0.269	−0.0062	28
0.4232	0.8321	1.43920	1262	754	0.297	−0.0063	30
0.4734	0.8350	1.44342	1261	753	0.312	−0.0066	33
0.5676	0.8406	1.45120	1261	749	0.337	−0.0072	36
0.6151	0.8436	1.45579	1261	746	0.339	−0.0068	37
0.6601	0.8466	1.45966	1261	742	0.329	−0.0070	38
0.7454	0.8526	1.46791	1264	734	0.291	−0.0063	36
0.7884	0.8558	1.47240	1267	728	0.262	−0.0057	34
0.8320	0.8591	1.47679	1270	722	0.233	−0.0052	30
0.8783	0.8628	1.48195	1275	713	0.189	−0.0041	25
0.9169	0.8660	1.48641	1281	703	0.146	−0.0031	19
0.9500	0.8688	1.49021	1288	694	0.108	−0.0023	12
1.0000	0.8736	1.49692	1299	678	0.000	0.0000	0
Cyclohexane (1) + 1-Pentanol (2)							
0.0492	0.8087	1.40777	1272	765	0.062	−0.008	4
0.0816	0.8072	1.40785	1269	769	0.102	−0.0012	7
0.1364	0.8048	1.40860	1264	777	0.150	−0.0013	11
0.1928	0.8025	1.40918	1260	785	0.177	−0.0016	15
0.2455	0.8002	1.40987	1256	792	0.222	−0.0017	18
0.2868	0.7986	1.41040	1254	797	0.231	−0.0018	21
0.3335	0.7965	1.41102	1251	803	0.280	−0.0019	24
0.4271	0.7926	1.41238	1244	815	0.338	−0.0020	30
0.5250	0.7887	1.41386	1239	825	0.374	−0.0020	34
0.6198	0.7850	1.41540	1236	833	0.398	−0.0020	36
0.6597	0.7835	1.41602	1236	835	0.401	−0.0019	35
0.7068	0.7818	1.41682	1236	838	0.394	−0.0019	35
0.7525	0.7803	1.41764	1236	839	0.366	−0.0018	33
0.8011	0.7787	1.41849	1236	840	0.337	−0.0017	31
0.8456	0.7774	1.41961	1238	839	0.288	−0.0012	27
0.8883	0.7761	1.42053	1240	838	0.247	−0.0010	23
0.9417	0.7748	1.42166	1244	834	0.151	−0.0006	15
1.0000	0.7737	1.42320	1254	822	0.000	0.0000	0

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Table 3. Densities, Refractive Indices, Speeds of Sound, Isentropic Compressibilities, Excess Molar Volumes, Changes of Refractive Index on Mixing, and Changes of Isentropic Compressibility on Mixing for Benzene (1) + Cyclohexane (2) + 1-Pentanol (3) at 298.15 K

x_1	x_2	ϱ/(g·cm^{-3})	n_D	u/(m·s^{-1})	κ_S/(TPa^{-1})	V_m^E/(cm^3·mol^{-1})	δn_D	$\delta\kappa_S$/(TPa^{-1})
0.0664	0.0458	0.8118	1.41210	1269	765	0.123	−0.0023	10
0.0631	0.2401	0.8031	1.41421	1254	792	0.284	−0.0029	24
0.0572	0.3482	0.7982	1.41540	1247	806	0.357	−0.0029	30
0.0620	0.6449	0.7864	1.41995	1234	834	0.478	−0.0033	40
0.0641	0.7366	0.7833	1.42198	1235	837	0.445	−0.0029	37
0.1783	0.0513	0.8170	1.42071	1264	766	0.194	−0.0038	19
0.1801	0.1393	0.8128	1.42133	1256	779	0.312	−0.0047	27
0.1746	0.2459	0.8076	1.42258	1248	795	0.418	−0.0046	35
0.1837	0.3355	0.8041	1.42424	1242	807	0.488	−0.0051	42
0.1796	0.5253	0.7957	1.42671	1234	826	0.609	−0.0052	49
0.1810	0.7091	0.7891	1.42979	1235	830	0.559	−0.0051	41
0.2942	0.1306	0.8187	1.43008	1253	779	0.395	−0.0060	36
0.2878	0.2369	0.8132	1.43064	1245	793	0.520	−0.0065	43
0.2904	0.3308	0.8089	1.43211	1238	806	0.618	−0.0067	50
0.2923	0.4191	0.8051	1.43345	1235	815	0.676	−0.0069	53
0.2954	0.5130	0.8015	1.43530	1234	820	0.687	−0.0067	53
0.2890	0.6098	0.7975	1.43647	1236	821	0.672	−0.0065	47
0.4057	0.1313	0.8243	1.43897	1250	777	0.481	−0.0070	43
0.4044	0.2272	0.8195	1.43992	1243	790	0.591	−0.0074	50
0.4028	0.3210	0.8150	1.44023	1238	800	0.673	−0.0084	54
0.4003	0.4077	0.8111	1.44241	1236	807	0.711	−0.0073	55
0.4021	0.4975	0.8075	1.44395	1238	808	0.725	−0.0073	50
0.5043	0.1135	0.8308	1.44737	1250	770	0.484	−0.0071	45
0.4939	0.2280	0.8244	1.44744	1243	785	0.619	−0.0079	52
0.4974	0.3141	0.8205	1.44905	1241	792	0.692	−0.0079	53
0.4945	0.3990	0.8168	1.45045	1241	794	0.702	−0.0076	50
0.5986	0.2219	0.8311	1.45676	1247	774	0.598	−0.0078	49
0.6902	0.0481	0.8461	1.46308	1259	746	0.378	−0.0070	40
0.6922	0.1290	0.8418	1.46426	1255	755	0.492	−0.0072	44
0.6865	0.2195	0.8371	1.46509	1255	759	0.550	−0.0073	42
0.7871	0.0401	0.8535	1.47233	1265	732	0.314	−0.0062	35
0.7764	0.1283	0.8480	1.47261	1264	739	0.421	−0.0064	35
0.8541	0.0488	0.8582	1.47981	1273	719	0.267	−0.0049	27
0.1223	0.0887	0.8125	1.41646	1263	771	0.203	−0.0036	18
0.4967	0.0626	0.8330	1.44619	1255	763	0.415	−0.0068	41
0.1835	0.4293	0.8000	1.42540	1237	817	0.553	−0.0054	47
0.0586	0.1432	0.8071	1.41269	1261	779	0.206	−0.0026	17
0.4663	0.4728	0.8122	1.44920	1243	797	0.704	−0.0074	46
0.8247	0.1198	0.8522	1.47787	1271	726	0.360	−0.0053	26
0.1312	0.2873	0.8038	1.41976	1247	800	0.415	−0.0042	34
0.8998	0.0475	0.8620	1.48572	1281	707	0.214	−0.0030	18

Table 4. Parameters A_{ij}, B_p, and C_i of Equations 1−3 and Standard Deviations σ

			Benzene (1) + 1-Pentanol (2)			
V_m^E/(cm^3·mol^{-1})	$B_0 = 1.3028$	$B_1 = 0.5605$	$B_2 = -0.3672$	$B_3 = -0.0551$	$B_4 = 0.9224$	$\sigma = 0.0041$
δn_D	$B_0 = -0.0273$	$B_1 = -0.0084$	$B_2 = -0.0084$			$\sigma = 0.0002$
$\delta\kappa_S$/(TPa^{-1})	$B_0 = 135.6$	$B_1 = 86.8$	$B_2 = 50.5$			$\sigma = 0.3$
			Cyclohexane (1) + 1-Pentanol (2)			
V_m^E/(cm^3·mol^{-1})	$B_0 = 1.4510$	$B_1 = 0.7922$	$B_2 = 0.5954$			$\sigma = 0.0081$
δn_D	$B_0 = -0.0080$	$B_1 = 0.0006$	$B_2 = -0.0059$			$\sigma = 0.0001$
$\delta\kappa_S$/(TPa^{-1})	$B_0 = 128.9$	$B_1 = 81.8$	$B_2 = 46.1$			$\sigma = 0.8$
			Benzene (1) + Cyclohexane (2) + 1-Pentanol (3)			
ϱ^{-1}/(g^{-1}·cm^3)	$A_{11} = 1.1685$	$A_{12} = -0.0111$	$A_{13} = -0.0246$	$A_{14} = 0.0121$		
	$A_{21} = 1.3083$	$A_{22} = -0.0183$	$A_{23} = 0.0075$	$A_{24} = -0.0049$		
	$A_{31} = 1.2445$	$A_{32} = -0.0471$	$A_{33} = 0.0554$	$A_{34} = -0.0196$		$\sigma = 0.0001$
n_D	$A_{11} = 1.4754$	$A_{12} = 0.0237$	$A_{13} = -0.0158$	$A_{14} = 0.0135$		
	$A_{21} = 1.4174$	$A_{22} = 0.0082$	$A_{23} = -0.0029$	$A_{24} = 0.0005$		
	$A_{31} = 1.3977$	$A_{32} = 0.0338$	$A_{33} = -0.0434$	$A_{34} = 0.0195$		$\sigma = 0.0002$
u/(m·s^{-1})	$A_{11} = 1248.20$	$A_{12} = 47.61$	$A_{13} = -0.57$	$A_{14} = 4.03$		
	$A_{21} = 1209.80$	$A_{22} = 36.56$	$A_{23} = 39.70$	$A_{24} = -32.94$		
	$A_{31} = 1104.50$	$A_{32} = 516.01$	$A_{33} = -557.74$	$A_{34} = 214.02$		$\sigma = 0.6$
κ_S/(TPa^{-1})	$A_{11} = 748.66$	$A_{12} = -53.79$	$A_{13} = -51.89$	$A_{14} = 35.13$		
	$A_{21} = 885.40$	$A_{22} = -50.35$	$A_{23} = -45.27$	$A_{24} = 33.18$		
	$A_{31} = 978.58$	$A_{32} = -667.03$	$A_{33} = 712.25$	$A_{34} = -267.24$		$\sigma = 0.7$
V_m^E/(cm^3·mol^{-1})	$C_1 = -0.9278$	$C_2 = 4.4454$	$C_3 = 5.8451$			$\sigma = 0.0075$
δn_D	$C_1 = 0.0401$	$C_2 = -0.0639$	$C_3 = -0.0756$			$\sigma = 0.0002$
$\delta\kappa_S$/(TPa^{-1})	$C_1 = -155.1$	$C_2 = 850.2$	$C_3 = 777.6$			$\sigma = 0.8$

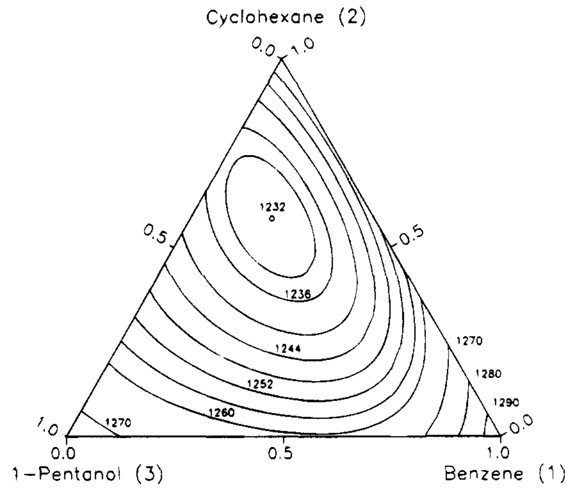

Figure 3. Speed of sound curves for benzene (1) + cyclohexane (2) + 1-pentanol (3) mixtures at 298.15 K.

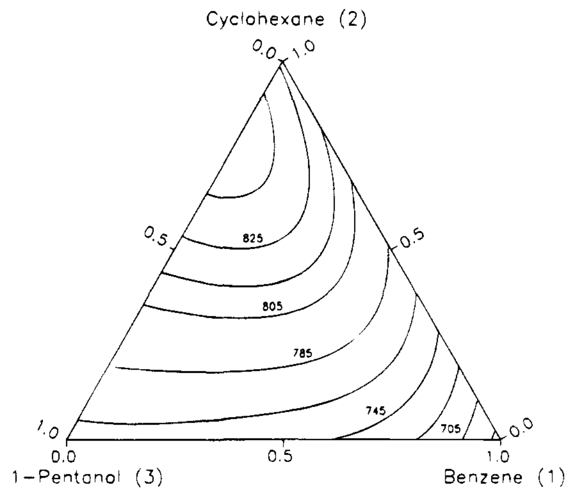

Figure 4. Isentropic compressibility curves for benzene (1) + cyclohexane (2) + 1−pentanol (3) mixtures at 298.15 K.

of aliphatic alcohols such as candidate entrainers for benzene−cyclohexane mixtures, knowledge of different physical properties is required to calculate bottom and head rectification compositions.

In previous papers (*1−3*) we presented densities and refractive indices for binary and ternary mixtures. In this paper we present densities, refractive indices, speeds of sound, and isentropic compressibilities at 298.15 K of benzene + cyclohexane + 1-pentanol and of the binary benzene + 1-pentanol and cyclohexane + 1-pentanol mixtures.

Experimental Section

Apparatus and Procedure. The densities and speeds of sound of the pure liquids and mixtures were measured with an Anton Paar DSA-48 density and sound analyzer with precisions of ±0.00005 g·cm^{-3} and ±1 m·s^{-1}, respectively, and the refractive indices by the automatic refractometer ABBEMAT-HP Dr Kernchen with a precision of ±0.00001. The experimental technique has been described previously (*1−3*).

Purity of Materials. Benzene, cyclohexane, and 1-pentanol were of Merck chromatographic grade. No further purification was attempted because the purity of materials had been previously checked by gas chromatography. The analysis showed that the major peak area exceeds 99.8% for benzene and cyclohexane and 99.4% for 1-pentanol. Table 1 compares some of the measured properties with the literature data.

Results and Discussion

Densities, refractive indices, speeds of sound, and isentropic compressibilities ($\kappa_S = \varrho^{-1}u^{-2}$) are given in Tables 2 and 3. These properties have been fitted to the Redlich−Kister (*11*) relation

$$Q = \sum_{i=1}^{3}\sum_{j=1}^{m} A_{ij}x_i^j \qquad (1)$$

where Q is u/(m·s^{-1}), ϱ^{-1}/(g^{-1}·cm^3), n_D, or κ_S/(TPa^{-1}) and x_i is the mole fraction of the component i. Figures 1, 2, 3, and 4 show, respectively, densities, refractive indices, speeds of sound, and isentropic compressibilities of the ternary mixture plotted against the mole fractions. Speed of sound curves presents a minimum at u = 1232 m·s^{-1}, whose coordinates are x_1 = 0.1885 and x_2 = 0.5753.

Excess molar volumes, changes of refractive indices on mixing and changes of isentropic compressibilities on mixing of the mixtures have been calculated from the expression:

$$\delta Q = x_i x_j \sum_{p=0}^{m} B_p(x_i - x_j)^p \qquad (2)$$

where δQ is V_m^E/(cm^3·mol^{-1}), δn_D, or $\delta\kappa_S$/(TPa^{-1}).

These physical properties of binary mixtures are listed in Table 2. Figure 5 shows the experimental points of V_m^E, δn_D, and $\delta\kappa_S$ plotted against x as well as the curves

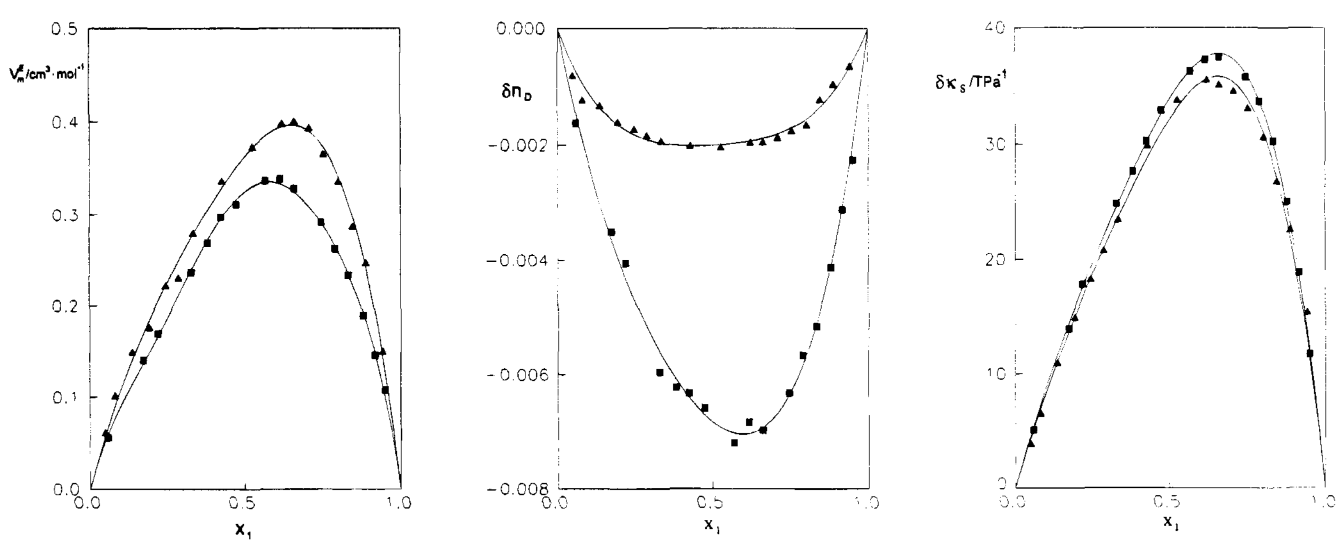

Figure 5. Variation of the (a, left) excess molar volumes, (b, middle) changes of refractive indices on mixing, and (c, right) changes of isentropic compressibilities on mixing with mole fraction at 298.15 K for (■) benzene (1) + 1-pentanol (2) and (▲) cyclohexane (1) + 1-pentanol (2).

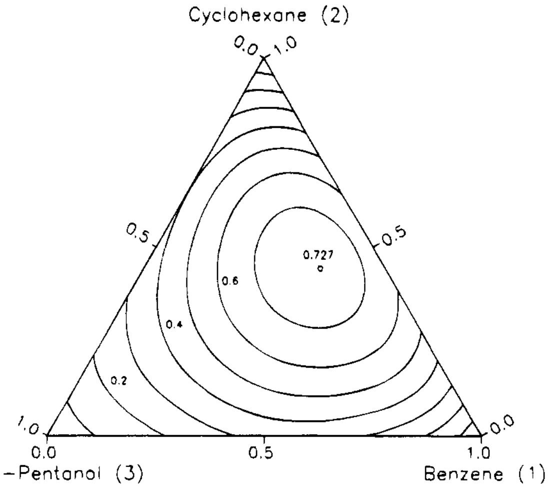

Figure 6. Excess molar volume curves for benzene (1) + cyclohexane (2) + 1-pentanol (3) mixtures at 298.15 K.

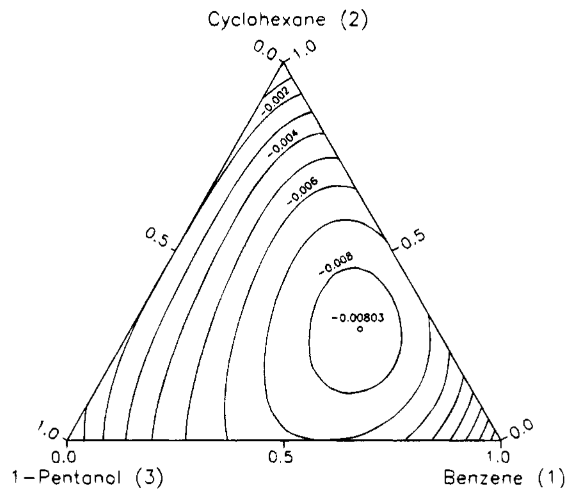

Figure 7. Changes of refractive index on mixing curves for benzene (1) + cyclohexane (2) + 1-pentanol (3) mixtures at 298.15 K.

fitted. Values of the binary mixture benzene + cyclohexane are available in previous work (*12*).

The experimental results of the ternary mixture are shown in Table 3. No values for this mixture have been found in previous papers. The results were correlated with the Cibulka (*13*) equation for the excess properties of the ternary mixtures

$$\delta Q_{123} = \delta Q_{bin} + x_1 x_2 (1 - x_1 - x_2)(C_1 + C_2 x_1 + C_3 x_2), \quad (3)$$

where

$$\delta Q_{bin} = \delta Q_{12} + \delta Q_{13} + \delta Q_{23} \quad (4)$$

The parameters A_{ij}, B_p, and C_i of eqs 1, 2, and 3, and corresponding standard deviations, are given in Table 4. An unweighted least-squares method was used to fit the polynomials of eqs 1−3 to the data. The degree of the eqs 1 and 2 was optimized by applying the F test (*14*).

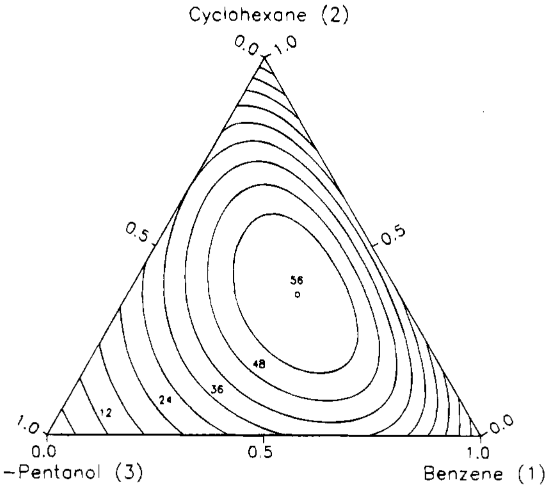

Figure 8. Changes of isentropic compressibility of mixing curves for benzene (1) + cyclohexane (2) + 1-pentanol (3) mixtures at 298.15 K.

Curves of constant V_m^E, δn_D, and $\delta \kappa_S$ (eq 3) have been plotted in Figures 6, 7, and 8, respectively, presenting V_m^E and $\delta \kappa_S$ a maximum at $V_m^E = 0.727$ cm^3·mol^{-1} in $x_1 = 0.4072$ and $x_2 = 0.4440$, and $\delta \kappa_S = 56$ TPa^{-1} in $x_1 = 0.3919$ and $x_2 = 0.3734$. Moreover, there is a minimum of changes of refractive index at $\delta n_D = -0.00803$ in $x_1 = 0.5292$ and $x_2 = 0.2942$.

Registry No. Supplied by the Author: Benzene, 71-43-2; cyclohexane, 110-82-7; 1-pentanol, 71-41-0.

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