Viscosities, Densities, and Speed of Sound of the Cycloalkanes with Secondary Alcohols at T = (293.15, 298.15, and 303.15) K: New UNIFAC−VISCO Interaction Parameters

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In this work, dynamic viscosities, densities, and speeds of sound have been measured over the whole composition range and at 0.1 MPa for binary mixtures (cyclopentane and cyclohexane with 2-propanol, 2-butanol, and 2-pentanol) at several temperatures T = (293.15, 298.15, and 303.15) K along with the properties of the pure components. Excess molar volumes, molar isentropic compressibilities, excess molar isentropic compressibilities, and viscosity deviations for the binary systems at the above-mentioned temperatures were calculated and fitted to the Redlich−Kister equation to determine the fitting parameters and the root-mean-square deviations. The UNIQUAC equation was used to correlate the experimental viscosity data. The UNIFAC−VISCO and ASOG−VISCO methods, which are based on contribution groups, were used to predict the dynamic viscosities of the binary mixtures. The interaction parameters of cycloalkanes with a secondary alcohol (CH_{cy}/OH_s) have been determined for their application in the predictive UNIFAC−VISCO method.

1. Introduction

Knowledge of the viscosity of liquid mixtures is very important for the design of processes for fluid transport not only through pipes but also through pore surfaces and in many process involving mass and energy transfer. As an extension of our work concerning the dynamic viscosity of binary systems of alkanes with alcohols,[1−3] in this paper we give experimental dynamic viscosity, density, and speed of sound data for cyclohexane (1) and cyclopentane (1) with 2-propanol (2) or 2-butanol (2) or 2-pentanol (2) at T = (293.15, 298.15, and 303.15) K. Lee and Chuang[4] and Gama and Tojo[5] have measured the excess molar volume of cyclohexane (1) with 2-propanol (2) and cyclohexane (1) with 2-butanol (2), respectively, and Gascón et al.[6] have measured the viscosity deviation of cyclohexane (1) with 2-butanol (2). Experimental data were used to calculate excess molar volumes, molar isentropic compressibilities, excess molar isentropic compressibilities, and viscosity deviations over the entire mole fraction range. Viscosity data were correlated using the UNIQUAC[7] equation.

The UNIFAC−VISCO[8,9] and ASOG−VISCO[10] methods have been applied to predict the viscosity of these systems, and the results were compared with the experimental data. To improve the results of the prediction of the UNIFAC−VISCO method, the interaction parameter CH_{cy}/OH_s has been determined.

2. Experimental Section

Chemicals. The pure components were supplied by Fluka (cyclohexane, cyclopentane) and Merck (2-propanol, 2-butanol, and 2-pentanol). The components were degassed ultrasonically and dried over type 4Å molecular sieves, which were supplied by Aldrich, and kept in inert argon with a maximum water mass fraction of 2×10^{-6}. The maximum water contents of the liquids were determined using a Metrohm 737 KF coulometer. Their mass fraction purities were >99.8 % for cyclohexane, >99.5 % for 2-butanol and 2-pentanol, >99.0 % for cyclopentane, and >99.7 % for 2-propanol.

Table 1. Comparison of Density ρ and Viscosity η with Literature Data for Pure Components at T = 298.15 K

	ρ/(g·cm^{-3})		$10^3\eta$/(Pa·s)	
component	exptl	lit	exptl	lit
cyclohexane	0.77392	0.7738[a]	0.887	0.888[a]
		0.77387[c]		0.883[b]
cyclopentane	0.73955	0.73969[d]	0.416	0.416[c]
		0.73947[e]		
2-propanol	0.78087	0.7809[f]	2.045	2.0436[c]
2-butanol	0.80272	0.8026[g]	2.995	2.998[g]
2-pentanol	0.80501	0.8050[h]	3.273	3.273[h]

[a] Petrino et al.[11] [b] Aminabhavi et al.[12] [c] Riddick et al.[13] [d] Guzman et al.[14] [e] Pereiro et al.[15] [f] Rodriguez et al.[16] [g] Das et al.[17] [h] González et al.[3]

Apparatus and Procedure. Samples were prepared by mass using a Mettler AX-205 Delta Range balance with a precision of $\pm 10^{-5}$ g, covering the whole composition range of the mixture.

Kinematic viscosities were determined using a Lauda PVS1 automatic viscosimeter with two Ubbelhode capillary microviscosimeters of 0.4 mm and 0.53 mm diameter. Gravity fall is the principle of measurement on which this viscosimeter is based. The capillary is maintained in a D20KP Lauda thermostat with a resolution of 0.01 K. The capillaries are calibrated and credited by the company. The uncertainty in the capillary diameter is ± 0.005 mm. To verify the calibration, the viscosity of the pure liquids was compared with recently published data (Table 1). The uncertainty in the viscosimeter measurement is ± 0.001 mPa·s. The equipment has a PVS1 control unit (Processor Viscosity System) that is a PC-controlled instrument for the precise measurement of fall time. It uses standardized glass capillaries and has an accuracy of 0.01 s.

The density and the speed of sound of the pure liquids and mixtures were measured using an Anton Paar DSA-5000 digital vibrating-tube densimeter. The uncertainty in the density

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Table 2. Density ρ, Speed of Sound u, Dynamic Viscosity η, Excess Molar Volumes V^E, Molar Isentropic Compressibility $K_{S,m}$, Excess Molar Isentropic Compressibility $K^E_{S,m}$, and Viscosity Deviations $\Delta\eta$ of Cyclohexane (1) + 2-Propanol (2)

x_1	ρ / g·cm^{-3}	u / m·s^{-1}	η / mPa·s	V^E / cm^3·mol^{-1}	$K_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$K^E_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$\Delta\eta$ / mPa·s
				$T = 293.15$ K			
0.0000	0.78507	1156	2.382	0.000	0.0729	0.0000	0.000
0.0484	0.78376	1160	2.184	0.087	0.0742	0.0005	−0.130
0.0970	0.78263	1163	1.988	0.162	0.0753	0.0009	−0.257
0.2006	0.78051	1171	1.651	0.304	0.0777	0.0018	−0.447
0.3002	0.77887	1180	1.427	0.416	0.0797	0.0024	−0.531
0.3977	0.77763	1189	1.264	0.496	0.0815	0.0029	−0.556
0.5070	0.77669	1200	1.128	0.544	0.0832	0.0033	−0.537
0.6046	0.77615	1211	1.025	0.555	0.0845	0.0035	−0.502
0.7058	0.77592	1223	0.969	0.531	0.0855	0.0034	−0.415
0.8230	0.77623	1240	0.944	0.429	0.0862	0.0029	−0.274
0.9016	0.77688	1254	0.950	0.298	0.0861	0.0021	−0.157
0.9521	0.77752	1265	0.962	0.181	0.0858	0.0014	−0.074
1.0000	0.77862	1279	0.968	0.000	0.0848	0.0000	0.000
				$T = 298.15$ K			
0.0000	0.78087	1139	2.045	0.000	0.0760	0.0000	0.000
0.0484	0.77950	1141	1.883	0.091	0.0774	0.0006	−0.105
0.0970	0.77829	1145	1.722	0.171	0.0787	0.0010	−0.211
0.2006	0.77605	1152	1.444	0.323	0.0813	0.0020	−0.369
0.3002	0.77429	1159	1.260	0.442	0.0836	0.0027	−0.438
0.3977	0.77295	1167	1.119	0.529	0.0856	0.0033	−0.466
0.5070	0.77192	1178	1.008	0.583	0.0875	0.0037	−0.450
0.6046	0.77134	1188	0.926	0.596	0.0889	0.0039	−0.419
0.7058	0.77111	1200	0.878	0.567	0.0900	0.0038	−0.350
0.8230	0.77142	1216	0.856	0.456	0.0907	0.0032	−0.236
0.9016	0.77209	1230	0.870	0.319	0.0907	0.0023	−0.131
0.9521	0.77274	1240	0.874	0.197	0.0904	0.0015	−0.068
1.0000	0.77392	1254	0.887	0.000	0.0893	0.0000	0.000
				$T = 303.15$ K			
0.0000	0.77660	1121	1.763	0.000	0.079	0.0000	0.000
0.0484	0.77515	1123	1.633	0.097	0.081	0.0006	−0.085
0.0970	0.77387	1126	1.504	0.182	0.082	0.0012	−0.167
0.2006	0.77150	1132	1.267	0.344	0.085	0.0022	−0.306
0.3002	0.76962	1139	1.112	0.473	0.088	0.0031	−0.367
0.3977	0.76819	1146	0.996	0.567	0.090	0.0037	−0.391
0.5070	0.76709	1155	0.908	0.625	0.092	0.0042	−0.375
0.6046	0.76647	1165	0.838	0.639	0.094	0.0044	−0.352
0.7058	0.76623	1176	0.798	0.606	0.095	0.0043	−0.296
0.8230	0.76656	1192	0.786	0.488	0.096	0.0036	−0.197
0.9016	0.76724	1206	0.801	0.343	0.096	0.0026	−0.108
0.9521	0.76792	1216	0.802	0.214	0.095	0.0017	−0.059
1.0000	0.76919	1230	0.816	0.000	0.094	0.0000	0.000

Table 3. Density ρ, Speed of Sound u, Dynamic Viscosity η, Excess Molar Volume V^E, Molar Isentropic Compressibility $K_{S,m}$, Excess Molar Isentropic Compressibility K^E_{Sm}, and Viscosities Deviations $\Delta\eta$ of Cyclohexane (1) + 2-Butanol (2)

x_1	ρ / g·cm^{-3}	u / m·s^{-1}	η / mPa·s	V^E / cm^3·mol^{-1}	$K_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$K^E_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$\Delta\eta$ / mPa·s
				$T = 293.15$ K			
0.0000	0.80684	1230	3.623	0.000	0.0752	0.0000	0.000
0.0494	0.80424	1228	3.231	0.113	0.0765	0.0005	−0.261
0.1003	0.80195	1226	2.915	0.189	0.0777	0.0009	−0.442
0.1969	0.79777	1223	2.227	0.328	0.0799	0.0018	−0.873
0.3052	0.79348	1222	1.726	0.457	0.0821	0.0026	−1.086
0.4044	0.78986	1222	1.480	0.554	0.0839	0.0032	−1.070
0.5004	0.78673	1224	1.315	0.616	0.0854	0.0037	−0.979
0.6016	0.78391	1228	1.160	0.632	0.0865	0.0039	−0.866
0.7145	0.78142	1236	1.066	0.576	0.0872	0.0036	−0.660
0.8067	0.77985	1245	0.980	0.477	0.0872	0.0031	−0.501
0.9046	0.77886	1259	0.962	0.285	0.0866	0.0020	−0.259
0.9523	0.77843	1267	0.993	0.185	0.0861	0.0014	−0.102
1.0000	0.77862	1279	0.968	0.000	0.0848	0.0000	0.000
				$T = 298.15$ K			
0.0000	0.80272	1212	2.995	0.000	0.0783	0.0000	0.000
0.0494	0.80004	1210	2.687	0.118	0.0797	0.0006	−0.203
0.1003	0.79769	1207	2.444	0.199	0.0810	0.0010	−0.339
0.1969	0.79337	1204	1.891	0.349	0.0835	0.0020	−0.689
0.3052	0.78895	1201	1.489	0.488	0.0859	0.0029	−0.863
0.4044	0.78524	1201	1.299	0.591	0.0880	0.0036	−0.844
0.5004	0.78204	1202	1.166	0.655	0.0896	0.0041	−0.774
0.6016	0.77918	1205	1.042	0.670	0.0909	0.0042	−0.685
0.7145	0.77668	1213	0.968	0.608	0.0916	0.0040	−0.521
0.8067	0.77508	1222	0.892	0.505	0.0917	0.0033	−0.403
0.9046	0.77406	1235	0.879	0.308	0.0911	0.0022	−0.209
0.9523	0.77365	1242	0.908	0.202	0.0906	0.0015	−0.080
1.0000	0.77392	1254	0.887	0.000	0.0893	0.0000	0.000
				$T = 303.15$ K			
0.0000	0.79851	1194	2.493	0.000	0.0815	0.0000	0.000
0.0494	0.79577	1191	2.251	0.123	0.0831	0.0006	−0.159
0.1003	0.79334	1188	2.066	0.211	0.0845	0.0012	−0.259
0.1969	0.78888	1184	1.623	0.372	0.0873	0.0022	−0.540
0.3052	0.78434	1181	1.294	0.520	0.0900	0.0032	−0.687
0.4044	0.78054	1179	1.142	0.629	0.0923	0.0040	−0.672
0.5004	0.77729	1180	1.042	0.695	0.0941	0.0045	−0.612
0.6016	0.77441	1183	0.942	0.708	0.0955	0.0046	−0.543
0.7145	0.77202	1189	0.888	0.623	0.0965	0.0044	−0.407
0.8067	0.77026	1198	0.817	0.536	0.0965	0.0036	−0.323
0.9046	0.76922	1211	0.806	0.333	0.0960	0.0024	−0.170
0.9523	0.76882	1218	0.833	0.221	0.0954	0.0016	−0.063
1.0000	0.76919	1230	0.816	0.000	0.0940	0.0000	0.000

Table 4. Density ρ, Speed of Sound u, Dynamic Viscosity η, Excess Molar Volume V^E, Molar Isentropic Compressibility $K_{S,m}$, Excess Molar Isentropic Compressibility $K^E_{S,m}$, and Viscosity Deviations $\Delta\eta$ of Cyclohexane (1) + 2-Pentanol (2)

x_1	ρ / g·cm^{-3}	u / m·s^{-1}	η / mPa·s	V^E / cm^3·mol^{-1}	$K_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$K^E_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$\Delta\eta$ / mPa·s
				$T = 293.15$ K			
0.0000	0.80904	1250	4.001	0.000	0.0862	0.0000	0.000
0.0495	0.80687	1247	3.606	0.091	0.0868	0.0007	−0.245
0.1002	0.80468	1244	3.195	0.181	0.0875	0.0014	−0.502
0.2019	0.80029	1238	2.516	0.360	0.0889	0.0029	−0.873
0.3067	0.79606	1234	1.922	0.506	0.0901	0.0042	−1.149
0.4011	0.79242	1231	1.583	0.614	0.0910	0.0052	−1.201
0.5085	0.78862	1230	1.317	0.689	0.0915	0.0059	−1.141
0.6066	0.78563	1232	1.170	0.692	0.0915	0.0060	−0.991
0.7118	0.78294	1239	1.067	0.623	0.0907	0.0053	−0.775
0.8096	0.78086	1247	1.045	0.497	0.0895	0.0043	−0.500
0.9049	0.77929	1259	1.009	0.312	0.0878	0.0028	−0.248
0.9557	0.77862	1267	0.997	0.189	0.0866	0.0017	−0.105
1.0000	0.77862	1279	0.968	0.000	0.0848	0.0000	0.000
				$T = 298.15$ K			
0.0000	0.80501	1232	3.273	0.000	0.0896	0.0000	0.000
0.0495	0.80277	1229	2.969	0.096	0.0904	0.0007	−0.186
0.1002	0.80052	1225	2.658	0.191	0.0912	0.0016	−0.376
0.2019	0.79600	1218	2.125	0.380	0.0928	0.0032	−0.666
0.3067	0.79167	1213	1.659	0.531	0.0942	0.0045	−0.883
0.4011	0.78798	1210	1.385	0.640	0.0952	0.0055	−0.931
0.5085	0.78411	1209	1.178	0.715	0.0959	0.0062	−0.881
0.6066	0.78109	1211	1.056	0.714	0.0959	0.0063	−0.770
0.7118	0.77832	1216	0.970	0.645	0.0952	0.0057	−0.605
0.8096	0.77618	1224	0.952	0.518	0.0941	0.0046	−0.390
0.9049	0.77454	1235	0.924	0.331	0.0924	0.0030	−0.190
0.9557	0.77386	1243	0.912	0.203	0.0911	0.0018	−0.081
1.0000	0.77392	1254	0.887	0.000	0.0893	0.0000	0.000
				$T = 303.15$ K			
0.0000	0.80090	1214	2.774	0.000	0.0933	0.0000	0.000
0.0495	0.79860	1210	2.474	0.102	0.0942	0.0008	−0.203
0.1002	0.79628	1206	2.237	0.202	0.0951	0.0017	−0.341
0.2019	0.79165	1199	1.820	0.399	0.0970	0.0034	−0.559
0.3067	0.78723	1193	1.441	0.556	0.0986	0.0048	−0.732
0.4011	0.78348	1189	1.233	0.665	0.0997	0.0059	−0.756
0.5085	0.77956	1187	1.058	0.741	0.1005	0.0066	−0.721
0.6066	0.77649	1189	0.957	0.738	0.1006	0.0066	−0.629
0.7118	0.77365	1194	0.885	0.669	0.1000	0.0060	−0.496
0.8096	0.77144	1201	0.871	0.541	0.0989	0.0048	−0.318
0.9049	0.76974	1211	0.845	0.352	0.0972	0.0032	−0.157
0.9557	0.76907	1219	0.837	0.218	0.0960	0.0019	−0.066
1.0000	0.76919	1230	0.816	0.000	0.0940	0.0000	0.000

Table 5. Density ρ, Speed of Sound u, Dynamic Viscosity η, Excess Molar Volume V^E, Molar Isentropic Compressibility $K_{S,m}$, Excess Molar Isentropic Compressibility $K^E_{S,m}$, and Viscosity Deviations $\Delta\eta$ of Cyclopentane (1) + 2-Propanol (2)

x_1	ρ / g·cm^{-3}	u / m·s^{-1}	η / mPa·s	V^E / cm^3· mol^{-1}	$K_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$K^E_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$\Delta\eta$ / mPa·s
				$T = 293.15$ K			
0.0000	0.78507	1156	2.382	0.000	0.0729	0.0000	0.000
0.0486	0.78253	1156	2.105	0.014	0.0740	0.0005	−0.183
0.0910	0.77996	1155	1.874	0.067	0.0752	0.0012	−0.331
0.2019	0.77433	1156	1.425	0.116	0.0775	0.0023	−0.564
0.2958	0.76922	1156	1.172	0.218	0.0797	0.0035	−0.635
0.3877	0.76463	1158	0.954	0.294	0.0815	0.0043	−0.674
0.4823	0.76038	1162	0.799	0.341	0.0831	0.0049	−0.646
0.5974	0.75559	1168	0.641	0.379	0.0847	0.0053	−0.580
0.7206	0.75097	1179	0.535	0.389	0.0858	0.0052	−0.447
0.8136	0.74796	1190	0.484	0.356	0.0860	0.0046	−0.318
0.9219	0.74539	1208	0.449	0.218	0.0853	0.0029	−0.141
0.9533	0.74487	1215	0.443	0.151	0.0849	0.0022	−0.087
1.0000	0.74452	1232	0.438	0.000	0.0832	0.0000	−0.001
				$T = 298.15$ K			
0.0000	0.78087	1139	2.045	0.000	0.0760	0.0000	0.000
0.0486	0.77824	1138	1.823	0.019	0.0773	0.0006	−0.143
0.0910	0.77560	1136	1.627	0.075	0.0785	0.0013	−0.270
0.2019	0.76977	1136	1.254	0.135	0.0812	0.0026	−0.462
0.2958	0.76452	1135	1.038	0.245	0.0837	0.0038	−0.525
0.3877	0.75981	1136	0.856	0.328	0.0858	0.0048	−0.557
0.4823	0.75545	1139	0.724	0.379	0.0876	0.0055	−0.535
0.5974	0.75058	1145	0.588	0.420	0.0894	0.0059	−0.484
0.7206	0.74592	1154	0.499	0.425	0.0907	0.0057	−0.372
0.8136	0.74289	1165	0.454	0.387	0.0910	0.0050	−0.266
0.9219	0.74033	1183	0.424	0.238	0.0903	0.0031	−0.119
0.9533	0.73986	1189	0.419	0.162	0.0898	0.0023	−0.073
1.0000	0.73955	1206	0.416	0.000	0.0880	0.0000	0.000
				$T = 303.15$ K			
0.0000	0.77660	1121	1.763	0.000	0.0792	0.0000	0.000
0.0486	0.77387	1120	1.587	0.025	0.0807	0.0007	−0.110
0.0910	0.77115	1118	1.421	0.085	0.0821	0.0014	−0.217
0.2019	0.76512	1116	1.110	0.158	0.0852	0.0029	−0.377
0.2958	0.75973	1114	0.925	0.275	0.0880	0.0043	−0.433
0.3877	0.75490	1114	0.770	0.366	0.0904	0.0053	−0.462
0.4823	0.75044	1116	0.658	0.423	0.0925	0.0061	−0.445
0.5974	0.74549	1121	0.542	0.465	0.0945	0.0065	−0.403
0.7206	0.74079	1130	0.466	0.466	0.0960	0.0064	−0.311
0.8136	0.73776	1140	0.427	0.421	0.0963	0.0055	−0.222
0.9219	0.73520	1157	0.401	0.262	0.0956	0.0035	−0.100
0.9533	0.73472	1164	0.398	0.185	0.0951	0.0026	−0.060
1.0000	0.73454	1180	0.394	0.000	0.0931	0.0000	0.000

Table 6. Density ρ, Speed of Sound u, Dynamic Viscosity η, Excess Molar Volume V^E, Molar Isentropic Compressibility $K_{S,m}$, Excess Molar Isentropic Compressibility $K^E_{S,m}$, and Viscosity Deviations $\Delta\eta$ of Cyclopentane (1) + 2-Butanol (2)

x_1	ρ / g·cm^{-3}	u / m·s^{-1}	η / mPa·s	V^E / cm^3· mol^{-1}	$K_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$K^E_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$\Delta\eta$ / mPa·s
				$T = 293.15$ K			
0.0000	0.80684	1230	3.623	0.000	0.0752	0.0000	0.000
0.0445	0.80352	1225	3.152	0.055	0.0763	0.0006	−0.330
0.1036	0.79950	1219	2.649	0.087	0.0775	0.0012	−0.645
0.1872	0.79375	1212	2.121	0.140	0.0793	0.0021	−0.906
0.2856	0.78701	1204	1.604	0.205	0.0812	0.0031	−1.110
0.3938	0.77961	1197	1.194	0.279	0.0833	0.0041	−1.175
0.4873	0.77326	1193	0.946	0.342	0.0848	0.0049	−1.125
0.6179	0.76492	1191	0.692	0.375	0.0863	0.0054	−0.964
0.7034	0.75979	1193	0.610	0.358	0.0868	0.0052	−0.774
0.8115	0.75371	1200	0.517	0.290	0.0865	0.0044	−0.522
0.9113	0.74861	1211	0.468	0.166	0.0856	0.0028	−0.254
0.9506	0.74674	1218	0.451	0.099	0.0849	0.0020	−0.145
1.0000	0.74452	1232	0.438	0.000	0.0832	0.0000	−0.001
				$T = 298.15$ K			
0.0000	0.80272	1212	2.995	0.000	0.0783	0.0000	0.000
0.0445	0.79933	1207	2.621	0.059	0.0795	0.0006	−0.259
0.1036	0.79520	1200	2.231	0.097	0.0809	0.0013	−0.497
0.1872	0.78932	1192	1.811	0.158	0.0829	0.0023	−0.701
0.2856	0.78242	1183	1.393	0.231	0.0851	0.0033	−0.866
0.3938	0.77487	1175	1.054	0.313	0.0874	0.0045	−0.925
0.4873	0.76843	1170	0.850	0.380	0.0892	0.0053	−0.888
0.6179	0.76001	1167	0.636	0.409	0.0909	0.0058	−0.765
0.7034	0.75484	1169	0.569	0.388	0.0915	0.0056	−0.612
0.8115	0.74871	1175	0.485	0.316	0.0914	0.0047	−0.417
0.9113	0.74357	1186	0.441	0.185	0.0905	0.0030	−0.204
0.9506	0.74170	1192	0.426	0.114	0.0898	0.0021	−0.118
1.0000	0.73955	1206	0.416	0.000	0.0880	0.0000	0.000
				$T = 303.15$ K			
0.0000	0.79851	1194	2.493	0.000	0.0815	0.0000	0.000
0.0445	0.79505	1188	2.194	0.063	0.0828	0.0007	−0.206
0.1036	0.79081	1181	1.898	0.108	0.0844	0.0014	−0.378
0.1872	0.78479	1172	1.560	0.177	0.0867	0.0025	−0.540
0.2856	0.77774	1162	1.219	0.260	0.0892	0.0036	−0.675
0.3938	0.77005	1153	0.940	0.349	0.0919	0.0049	−0.727
0.4873	0.76352	1148	0.770	0.419	0.0939	0.0058	−0.700
0.6179	0.75502	1144	0.588	0.446	0.0959	0.0063	−0.608
0.7034	0.74982	1145	0.531	0.422	0.0966	0.0061	−0.485
0.8115	0.74364	1151	0.455	0.345	0.0967	0.0051	−0.335
0.9113	0.73846	1161	0.416	0.208	0.0957	0.0033	−0.164
0.9506	0.73660	1167	0.403	0.132	0.0950	0.0023	−0.095
1.0000	0.73454	1180	0.394	0.000	0.0931	0.0000	0.000

Table 7. Density ρ, Speed of Sound u, Dynamic Viscosity η, Excess Molar Volume V^E, Molar Isentropic Compressibiltiy $K_{S,m}$, Excess Molar Isentropic Compressibility $K^E_{S,m}$, and Viscosity Deviations $\Delta\eta$ of Cyclopentane (1) + 2-Pentanol (2)

x_1	ρ / g·cm^{-3}	u / m·s^{-1}	η / mPa·s	V^E / cm^3· mol^{-1}	$K_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$K^E_{S,m}$ / m^3·TPa^{-1}·mol^{-1}	$\Delta\eta$ / mPa·s
				$T = 293.15$ K			
0.0000	0.80904	1250	4.001	0.000	0.0862	0.0000	0.000
0.0450	0.80638	1246	3.573	0.019	0.0866	0.0005	−0.268
0.1030	0.80280	1239	3.005	0.056	0.0872	0.0014	−0.629
0.1878	0.79738	1229	2.322	0.123	0.0882	0.0026	−1.010
0.2924	0.79057	1218	1.723	0.200	0.0893	0.0040	−1.237
0.3906	0.78389	1209	1.296	0.286	0.0902	0.0052	−1.313
0.5117	0.77568	1201	0.957	0.355	0.0909	0.0063	−1.221
0.6242	0.76816	1197	0.747	0.372	0.0908	0.0065	−1.031
0.7210	0.76181	1198	0.629	0.346	0.0901	0.0061	−0.803
0.8091	0.75627	1202	0.552	0.269	0.0889	0.0051	−0.567
0.9094	0.74982	1211	0.482	0.175	0.0869	0.0035	−0.280
0.9552	0.74694	1218	0.455	0.115	0.0856	0.0023	−0.143
1.0000	0.74452	1232	0.439	0.000	0.0832	0.0000	0.000
				$T = 298.15$ K			
0.0000	0.80501	1232	3.273	0.000	0.0896	0.0000	0.000
0.0450	0.80228	1227	2.948	0.023	0.0901	0.0006	−0.197
0.1030	0.79862	1220	2.509	0.065	0.0909	0.0015	−0.469
0.1878	0.79307	1209	1.969	0.139	0.0921	0.0028	−0.768
0.2924	0.78612	1198	1.491	0.223	0.0935	0.0043	−0.947
0.3906	0.77933	1188	1.148	0.312	0.0946	0.0056	−1.009
0.5117	0.77103	1179	0.870	0.379	0.0954	0.0067	−0.941
0.6242	0.76343	1175	0.694	0.393	0.0955	0.0069	−0.795
0.7210	0.75698	1175	0.587	0.367	0.0949	0.0065	−0.626
0.8091	0.75136	1178	0.516	0.289	0.0938	0.0055	−0.445
0.9094	0.74482	1186	0.453	0.192	0.0918	0.0037	−0.222
0.9552	0.74192	1193	0.430	0.128	0.0905	0.0024	−0.114
1.0000	0.73955	1206	0.416	0.000	0.0880	0.0000	0.000
				T = 303.15 K			
0.0000	0.80090	1214	2.774	0.000	0.0933	0.0000	0.000
0.0450	0.79810	1208	2.459	0.027	0.0939	0.0006	−0.208
0.1030	0.79435	1200	2.118	0.074	0.0949	0.0016	−0.410
0.1878	0.78868	1189	1.687	0.156	0.0963	0.0030	−0.640
0.2924	0.78160	1177	1.304	0.245	0.0979	0.0046	−0.774
0.3906	0.77471	1167	1.027	0.337	0.0992	0.0060	−0.817
0.5117	0.76632	1157	0.794	0.403	0.1003	0.0071	−0.762
0.6242	0.75863	1152	0.645	0.415	0.1005	0.0073	−0.644
0.7210	0.75209	1152	0.548	0.389	0.1001	0.0069	−0.510
0.8091	0.74638	1154	0.487	0.312	0.0990	0.0059	−0.361
0.9094	0.73976	1161	0.428	0.212	0.0971	0.0040	−0.182
0.9552	0.73685	1167	0.407	0.144	0.0957	0.0026	−0.094
1.0000	0.73454	1180	0.394	0.000	0.0931	0.0000	0.000

Table 8. Fitting Parameters, Root-Mean-Square Deviation σ, and Estandard Error EE for Binary Mixtures at T = (273.15, 298.15, and 303.15) K

Cyclohexane (1) + 2-Propanol (2)						
$T = 293.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 2.1575$	$B_1 = 0.5965$	$B_2 = 0.6909$	$B_3 = 0.5730$	$\sigma = 0.005$	EE = 0.001
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0131$	$B_1 = 0.0050$	$B_2 = 0.0065$	$B_3 = 0.0056$	$\sigma = 0.00006$	EE = 1.7×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -2.1985$	$B_1 = 0.6912$	$B_2 = -0.2837$		$\sigma = 0.007$	EE = 0.002
$T = 298.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 2.3082$	$B_1 = 0.6448$	$B_2 = 0.7128$	$B_3 = 0.6310$	$\sigma = 0.007$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0147$	$B_1 = 0.0056$	$B_2 = 0.0068$	$B_3 = 0.0057$	$\sigma = 0.00007$	EE = 1.9×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -1.8380$	$B_1 = 0.5282$	$B_2 = -0.2365$		$\sigma = 0.006$	EE = 0.002
$T = 303.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 2.4723$	$B_1 = 0.6818$	$B_2 = 0.7548$	$B_3 = 0.7269$	$\sigma = 0.007$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0166$	$B_1 = 0.0061$	$B_2 = 0.0071$	$B_3 = 0.0063$	$\sigma = 0.00007$	EE = 1.9×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -1.5464$	$B_1 = 0.4166$	$B_2 = -0.1383$		$\sigma = 0.006$	EE = 0.002
Cyclohexane (1) + 2-Butanol (2)						
$T = 293.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 2.4704$	$B_1 = 0.8165$	$B_2 = -0.1883$	$B_3 = -0.0312$	$B_4 = 1.0803$	$\sigma = 0.006$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0145$	$B_1 = 0.0073$	$B_2 = 0.0036$			$\sigma = 0.00009$	EE = 2.5×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -3.9455$	$B_1 = 2.4492$	$B_2 = -2.1833$	$B_3 = -1.5063$	$B_4 = 3.0778$	$\sigma = 0.017$	EE = 0.005
$T = 298.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 2.6260$	$B_1 = 0.8044$	$B_2 = -0.2667$	$B_3 = 0.1273$	$B_4 = 1.2915$	$\sigma = 0.006$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0160$	$B_1 = 0.0077$	$B_2 = 0.0036$			$\sigma = 0.00010$	EE = 2.8×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -3.1142$	$B_1 = 1.9600$	$B_2 = -1.8395$	$B_3 = -1.3380$	$B_4 = 2.6414$	$\sigma = 0.015$	EE = 0.004
$T = 303.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 2.7859$	$B_1 = 0.7064$	$B_2 = -0.4864$	$B_3 = 0.4438$	$B_4 = 1.7499$	$\sigma = 0.008$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0177$	$B_1 = 0.0083$	$B_2 = 0.0039$			$\sigma = 0.00010$	EE = 2.8×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -2.4703$	$B_1 = 1.6096$	$B_2 = -1.4295$	$B_3 = -1.2734$	$B_4 = 2.1132$	$\sigma = 0.014$	EE = 0.004
Cyclohexane (1) + 2-Pentanol (2)						
$T = 293.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 2.7424$	$B_1 = 0.7012$	$B_2 = -0.4902$	$B_3 = 0.5131$	$B_4 = 1.0543$	$\sigma = 0.007$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0230$	$B_1 = 0.0086$	$B_2 = 0.0011$			$\sigma = 0.00012$	EE = 3.3×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -4.6171$	$B_1 = 2.0754$	$B_2 = 0.2151$	$B_3 = -0.7033$	$B_4 = 0.7946$	$\sigma = 0.009$	EE = 0.002
$T = 298.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 2.8595$	$B_1 = 0.6624$	$B_2 = -0.5012$	$B_3 = 0.6922$	$B_4 = 1.2155$	$\sigma = 0.007$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0244$	$B_1 = 0.0089$	$B_2 = 0.0015$			$\sigma = 0.00013$	EE = 3.6×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -3.5788$	$B_1 = 1.5500$	$B_2 = 0.1951$	$B_3 = -0.5600$	$B_4 = 0.7182$	$\sigma = 0.006$	EE = 0.002
$T = 303.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 2.9623$	$B_1 = 0.6238$	$B_2 = -0.4563$	$B_3 = 0.8808$	$B_4 = 1.3470$	$\sigma = 0.008$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0258$	$B_1 = 0.0092$	$B_2 = 0.0022$			$\sigma = 0.00015$	EE = 4.2×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -2.9268$	$B_1 = 1.1809$	$B_2 = 0.2919$	$B_3 = 0.1266$	$B_4 = -0.2099$	$\sigma = 0.009$	EE = 0.002
Cyclopentane (1) + 2-Propanol (2)						
$T = 293.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 1.4108$	$B_1 = 0.9029$	$B_2 = 0.0895$	$B_3 = 0.8201$	$B_4 = 0.6941$	$\sigma = 0.008$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0197$	$B_1 = 0.0086$	$B_2 = 0.0085$	$B_3 = 0.0110$		$\sigma = 0.00011$	EE = 3.1×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -2.5648$	$B_1 = 1.1101$	$B_2 = -0.6093$			$\sigma = 0.007$	EE = 0.002
$T = 298.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 1.5672$	$B_1 = 0.9520$	$B_2 = 0.0612$	$B_3 = 0.8762$	$B_4 = 0.7872$	$\sigma = 0.008$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0219$	$B_1 = 0.0096$	$B_2 = 0.0088$	$B_3 = 0.0114$		$\sigma = 0.00012$	EE = 3.3×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -2.1310$	$B_1 = 0.8762$	$B_2 = -0.4603$			$\sigma = 0.006$	EE = 0.001
$T = 303.15$ K						
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 1.7442$	$B_1 = 0.9833$	$B_2 = -0.0183$	$B_3 = 1.0266$	$B_4 = 1.0333$	$\sigma = 0.007$	EE = 0.001
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0243$	$B_1 = 0.0105$	$B_2 = 0.0095$	$B_3 = 0.0126$		$\sigma = 0.00013$	EE = 3.6×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -1.7770$	$B_1 = 0.6838$	$B_2 = -0.3083$			$\sigma = 0.005$	EE = 0.002

Table 8. (Continued)

Cyclopentane (1) + 2-Butanol (2)							
$T = 293.15$ K							
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 1.3592$	$B_1 = 0.9510$	$B_2 = 0.1821$	$B_3 = -0.4622$		$\sigma = 0.005$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0195$	$B_1 = 0.0125$	$B_2 = 0.0061$			$\sigma = 0.00011$	EE = 3.1×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -4.4948$	$B_1 = 1.8379$	$B_2 = -0.0575$	$B_3 = 0.7892$	$B_4 = -1.2587$	$\sigma = 0.007$	EE = 0.002
$T = 298.15$ K							
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 1.5003$	$B_1 = 0.9407$	$B_2 = 0.2110$	$B_3 = -0.3168$		$\sigma = 0.006$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0211$	$B_1 = 0.0133$	$B_2 = 0.0060$			$\sigma = 0.00012$	EE = 3.3×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -3.5554$	$B_1 = 1.3786$	$B_2 = 0.1322$	$B_3 = 0.5818$	$B_4 = -1.1794$	$\sigma = 0.006$	EE = 0.002
$T = 303.15$ K							
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 1.6495$	$B_1 = 0.9288$	$B_2 = 0.2648$	$B_3 = -0.1363$		$\sigma = 0.008$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0229$	$B_1 = 0.0143$	$B_2 = 0.0065$			$\sigma = 0.00013$	EE = 3.6×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -2.8097$	$B_1 = 1.0149$	$B_2 = 0.2350$	$B_3 = 0.4280$	$B_4 = -1.0470$	$\sigma = 0.006$	EE = 0.002
Cyclopentane (1) + 2-Pentanol (2)							
$T = 293.15$ K							
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 1.4136$	$B_1 = 0.7678$	$B_2 = -0.6889$	$B_3 = 0.2642$	$B_4 = 0.9566$	$\sigma = 0.007$	EE = 0.002
$K^E_{Sm}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0249$	$B_1 = 0.0105$	$B_2 = -0.0049$	$B_3 = 0.0098$	$B_4 = 0.0161$	$\sigma = 0.00009$	EE = 2.5×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -4.9373$	$B_1 = 2.5292$	$B_2 = -0.8087$	$B_3 = -0.7093$	$B_4 = 0.9325$	$\sigma = 0.009$	EE = 0.002
Cyclopentane (1) + 2-Pentanol (2)							
$T = 298.15$ K							
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 1.5111$	$B_1 = -0.7227$	$B_2 = -0.6762$	$B_3 = 0.4384$	$B_4 = 1.0670$	$\sigma = 0.007$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0265$	$B_1 = 0.0108$	$B_2 = -0.0046$	$B_3 = 0.0108$	$B_4 = 0.0164$	$\sigma = 0.00008$	EE = 2.2×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -3.7997$	$B_1 = 1.9133$	$B_2 = -0.6897$	$B_3 = -0.7234$	$B_4 = 0.9136$	$\sigma = 0.007$	EE = 0.002
$T = 303.15$ K							
$V^E/(cm^3 \cdot mol^{-1})$	$B_o = 1.6096$	$B_1 = 0.6822$	$B_2 = -0.6467$	$B_3 = 0.6322$	$B_4 = 1.2015$	$\sigma = 0.007$	EE = 0.002
$K^E_{S,m}/(m^3 \cdot TPa^{-1} \cdot mol^{-1})$	$B_o = 0.0281$	$B_1 = 0.0111$	$B_2 = -0.0041$	$B_3 = 0.0122$	$B_4 = 0.0171$	$\sigma = 0.00008$	EE = 2.2×10^{-5}
$\Delta\eta/(mPa \cdot s)$	$B_o = -3.0856$	$B_1 = 1.4613$	$B_2 = -0.3994$	$B_3 = -0.0319$	$B_4 = -0.0680$	$\sigma = 0.003$	EE = 0.001

Table 9. UNIQUAC Parameters and the Objective Function OF

systems	$\tau_{12}/(J \cdot mol^{-1})$	$\tau_{21}/(J \cdot mol^{-1})$	OF
cyclohexane (1) + 2-propanol (2)	65.76	143.75	0.171
cyclohexane (1) + 2-butanol (2)	249.62	−36.25	0.613
cyclohexane (1) + 2-pentanol (2)	204.33	18.12	0.784
cyclopentane (1) + 2-propanol (2)	−96.57	285.63	0.179
cyclopentane (1) + 2-butanol (2)	43.51	173.32	0.371
cyclopentane (1) + 2-pentanol (2)	91.36	76.66	0.388

Table 10. Experimental Data Used for Calculating New Interaction Parameters

binary systems	range T/K	no. of data points	interaction parameters
cyclohexane with 2-propanol, 2-butanol, 2-pentanol[a]	293.15−303.15	117	
cyclopentane with 2-propanol, 2-butanol, 2-pentanol[a]	293.15−303.15	117	CH_{cy}/OH_S
methylcyclopentane with 2-propanol, 2-butanol, 2-pentanol[b]	293.15−303.15	117	

[a] In this paper. [b] González et al.[24]

Table 11. New UNIFAC−VISCO Interaction Parameters

α_{mn}	$-CH_2-$	CH_3-	CH_{cy}	$-OH_S-$
$-CH_2-$	194.26	185.70	185.70	1197.53
CH_3-	−872.51	0	484.69	3957.26
CH_{cy}	−625.25	−225.37	0	711.75
$-OH_S-$	5872.78	−214.08	−77.02	0

measurement is $\pm 2 \times 10^{-6}$ g·cm^{-3}, and for the speed of sound, the uncertainty is $\pm$ 0.1 m·s^{-1}. The accuracy and precision are $\pm 10^{-6}$ g·cm^{-3} and $\pm 2 \times 10^{-6}$ g·cm^{-3} for the density and $\pm$ 0.1 m·s^{-1} and $\pm 10^{-2}$m·s^{-1} for the speed of sound, respectively.

3. Results and Discussion

The dynamic viscosity, density, speed of sound, excess molar volume, and viscosity deviation for the systems cyclohexane (1) and cyclopentane (1) with 2-propanol (2), 2-butanol (2), and 2-pentanol (2) at T = (293.15, 298.15, and 303.15) K and atmospheric pressure are reported in Tables 2 to 7. The excess molar volumes and viscosity deviations were calculated by the following equations

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

$$\Delta\eta = \eta - \sum_{i}^{N} x_i \eta_i \quad (2)$$

where ρ and ρ_i are the density of the mixture and the density of the pure components, respectively; x_i represents the mole fraction of component i; and η and η_i are the dynamic viscosity of the mixture and the pure component, respectively.

The speed of sound u is related to the isentropic compressibility k_s by the Laplace equation

$$\kappa_s = -V_m^{-1}\left(\frac{\partial V_m}{\partial \rho}\right)_S = \rho^{-1}u^{-2} = \frac{V_m}{M_m u^2} \quad (3)$$

where V_m is the molar volume and M_m is the molar mass of the mixture.

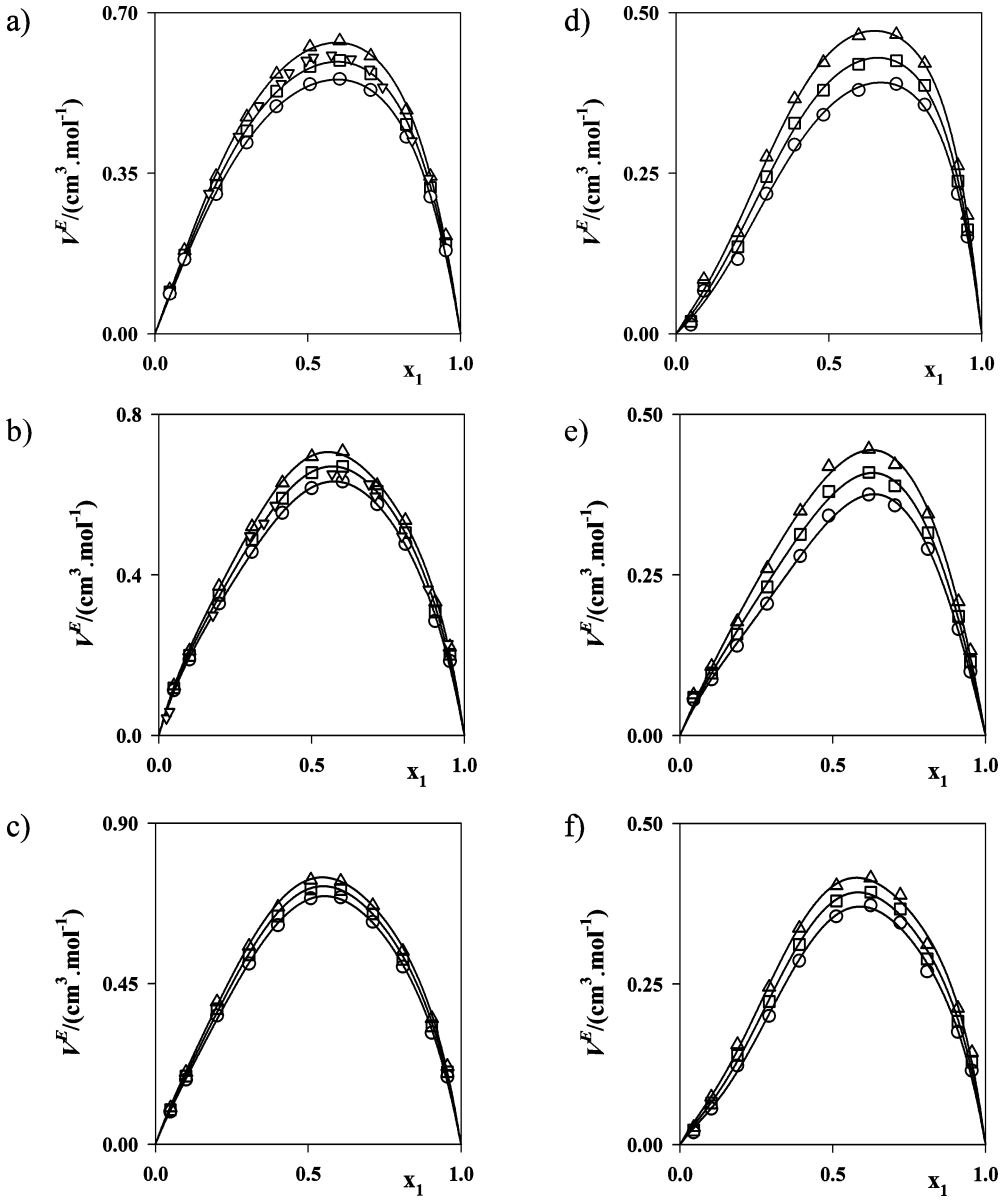

Figure 1. Excess molar volume, V^E, from the Redlich−Kister equation (−) plotted against mole fraction at T = 293.15 K (○), T = 298.15 K (□), and T = 313.15 K (△), for the binary mixtures (a) cyclohexane (1) + 2-propanol (2) and Lee et al. (▽, 298.15 K), (b) cyclohexane (1) + 2-butanol (2) and Gama et al. (▽, 298.15 K), (c) cyclohexane (1) + 2-pentanol (2), (d) cyclopentane (1) + 2-propanol (2), (e) cyclopentane (1) + 2-butanol (2), and (f) cyclopentane (1) + 2-pentanol (2).

To agree with the other thermodynamic quantities, it is appropriate to shift from the volume-intensive k_s to the molein-tensive $K_{S,m}$ (Douheret et al.[18,19])

$$K_{S,m} = -\left(\frac{\partial V_m}{\partial \rho}\right)_S = V_m \kappa_s = \frac{{V_m}^2}{M_m u^2} \tag{4}$$

where $K_{S,m}$ is the molar isentropic compressibility.

Experimental values for the speed of sound are reported in Tables 2 through 7 together with derived values of the molar isentropic compressibility and its excess, $K^E_{S,m}$. The excess molar isentropic compressibility $K^E_{S,m}$ is calculated by the following equation

$$K^E_{S,m} = K_{S,m} - K^{id}_{S,m} \tag{5}$$

where $K^{id}_{S,m}$ is defined by the approach developed by Benson and Kiyohara[20]

$$K^{id}_{S,m} = \sum_i x_i \left[K^*_{S,i} + T\frac{(E^*_{p,i})^2}{C^*_{p,i}}\right] - T\left[\frac{(\sum_i x_i E^*_{p,i})^2}{\sum_i x_i C^*_{p,i}}\right] \tag{6}$$

and $K^*_{S,i}$ is the product of the molar volume V^*_i and the isentropic compressibility $\kappa^*_{S,i}$ of pure component i. The molar isobaric expansion of pure component i, $E^*_{p,i}$, is the product of the molar volume and the isobaric expansibility $\alpha^*_{p,i}$, and $C^*_{p,i}$ is the molar isobaric heat capacity of pure component i.

The binary deviations at several temperatures were fitted to a Redlich−Kister[21]-type equation

$$\Delta Q_{12} = x_1 x_2 \sum_{p=0}^{M} B_p (x_1 - x_2)^p \tag{7}$$

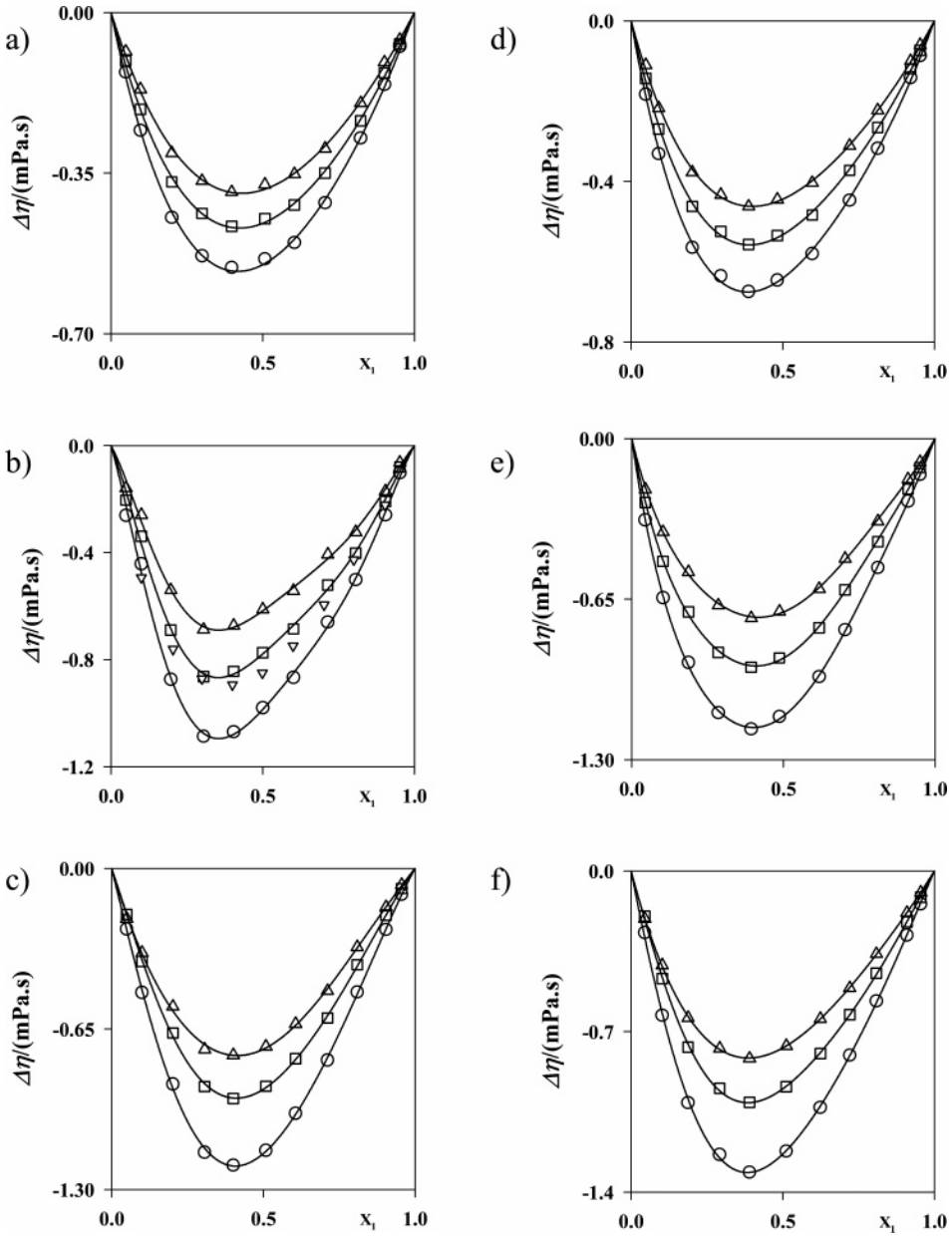

Figure 2. Viscosities deviations, $\Delta\eta$, from the Redlich−Kister equation (—) plotted against mole fraction at $T = 293.15$ K (○), $T = 298.15$ K (□) and $T = 313.15$ K (△), for the binary mixtures (a) cyclohexane (1) + 2-propanol (2) and (b) cyclohexane (1) + 2-butanol (2) and Gascón et al. (▽, 298.15 K), (c) cyclohexane (1) + 2-pentanol (2), (d) cyclopentane (1) + 2-propanol (2), (e) cyclopentane (1) + 2-butanol (2), and (f) cyclopentane (1) + 2-pentanol (2).

where ΔQ_{12} is the excess property, x_1 and x_2 are the mole fractions of component 1 and 2, respectively, B_P is the fitting parameter, and M is the degree of the polynomic expansion, which was optimized using the F test.[22] The fitting parameters are given in Table 8 together with the root-mean-square deviations σ (eq 8) and the standard error EE (eq 9)

$$\sigma = \left\{ \frac{\sum_{i}^{n_{dat}} (z_{exptl} - z_{calcd})^2}{n_{dat}} \right\}^{1/2} \tag{8}$$

$$EE = \frac{\sigma}{(n_{dat})^{1/2}} \tag{9}$$

where z_{exptl}, z_{calcd}, and n_{dat} are the values of the experimental and calculated properties and the number of experimental data points, respectively.

Figures 1 and 2 show the fitted curves as well as excess and deviation values of the systems cyclohexane (1) and cyclopentane (1) with 2-propanol (2), 2-butanol (2), and 2-pentanol (2) at $T =$ (293.15, 298.15, and 303.15) K. In Figure 1, the literature values of the cyclopentane (1) + 2-propanol (2) mixture of Lee et al. and cyclopentane (1) + 2-butanol (2) mixture of Gama et al. at 298.15 K are also shown. All systems present similar behavior for these physical properties.

As we can observe, in Figure 1, the excess molar volumes is positive over the entire composition range for the six investigated mixtures, with a maximum over $x_1 = 0.6$ except for cyclopentane (1) with 2-propanol (2), which presents it over $x_1 = 0.7$. The positive deviations of the excess molar volumes increase with the increase in temperature for all studied systems. For the systems cyclohexane with secondary alcohols, the excess molar volume increases with the increasing chain length of the alcohol, and this increase implies that dipole−dipole interactions are weak in higher 2-alkanol owing to the decrease in their polarizability with increasing chain length (Al-Hayan et al.[23]). For the systems with cyclopentane in which the excess molar volume decreases slightly with the increasing chain length

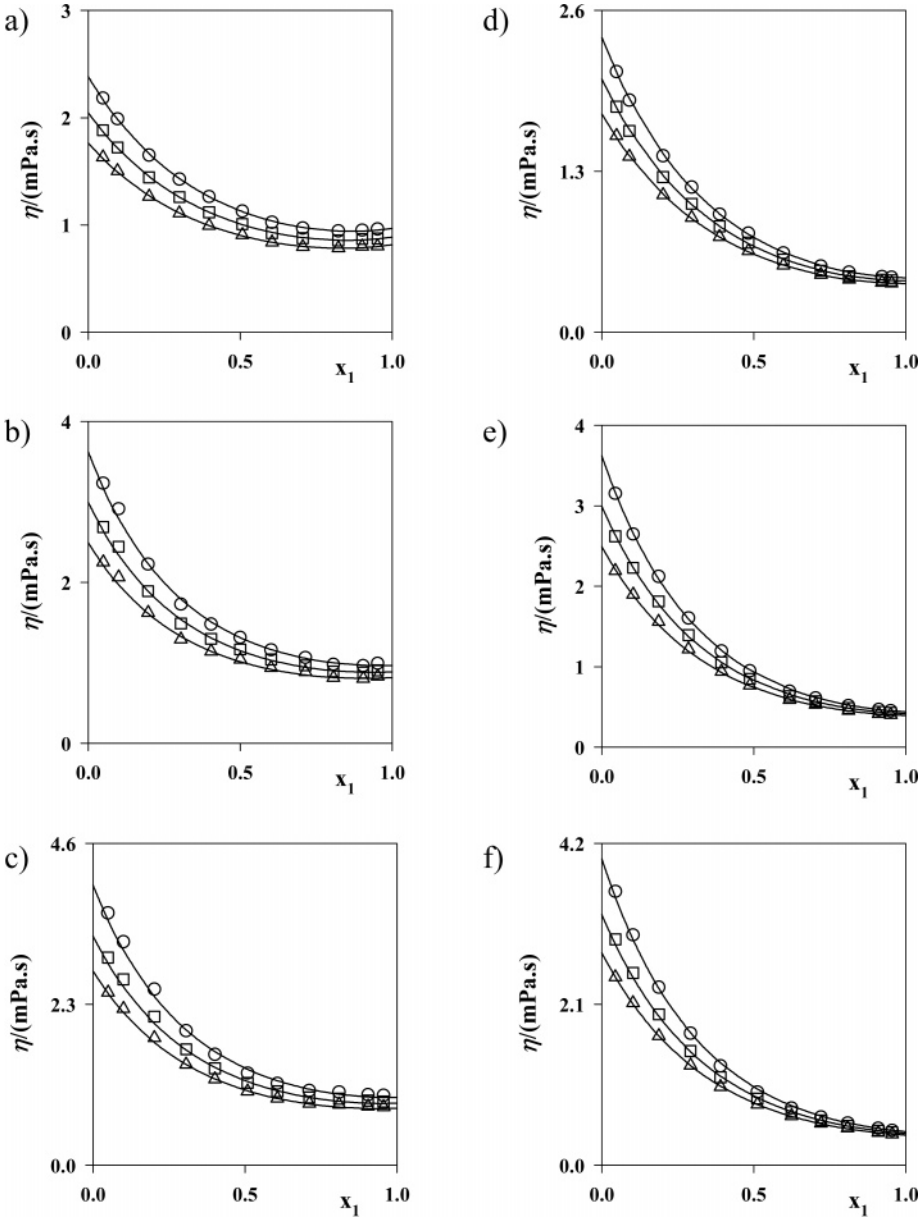

Figure 3. Dynamic viscosity, η, from the UNIQUAC equation (−) plotted against mole fraction at $T = 293.15$ K (○), $T = 298.15$ K (□), and $T = 313.15$ K (△) for the binary mixtures (a) cyclohexane (1) + 2-propanol (2) and (b) cyclohexane (1) + 2-butanol (2), (c) cyclohexane (1) + 2-pentanol (2), (d) cyclopentane (1) + 2-propanol (2), (e) cyclopentane (1) + 2-butanol (2), and (f) cyclopentane (1) + 2-pentanol (2).

of alcohols, the dipole−dipole interaction are stronger in higher 2-alkanols. However, the positive deviations increase with the increasing chain length of the cycloalkane.

In Figure 2, for viscosity deviations, the sign is negative for all systems with a minimum over $x_1 = 0.4$ except for cyclohexane (1) with 2-butanol (2), where the minimum lies at approximately $x_1 = 0.3$ mole fraction. For all systems under study, the negative deviation in viscosity increases when the chain length of the alcohol increase and with decreasing temperature. Indeed, the negative deviation decreases with the increase in the chain length of the cycloalkane. In this Figure, the literature values of cyclopentane (1) with 2-butanol (2) of Gascón et al. at 298.15 K are also shown.

4. Correlation and Prediction

The UNIQUAC[4] equation is used for calculating of the excess molar free energy of activation for flow, ΔG^{*E}, which is related to the viscosity by

$$\ln(\nu M) = \sum_i x_i \ln(\nu_i M_i) + \frac{\Delta G^{*E}}{RT} \tag{10}$$

where ν is the kinematic viscosity and M and M_i are the molecular weight of the mixture and the pure component, respectively.

The correlation has been performed with experimental data using the UNIQUAC equation to calculate the excess molar free energy by minimizing the following objective function

$$\mathrm{OF} = \frac{1}{N}\sum_{i=1}^{N}\frac{|\eta_{i,\mathrm{exptl}} - \eta_{i,\mathrm{calcd}}|}{\eta_{i,\mathrm{exptl}}} \tag{11}$$

where N is the number of experimental data and $\eta_{i,\mathrm{exptl}}$ and $\eta_{i,\mathrm{calcd}}$ are the experimental and calculated dynamic viscosity, respec-

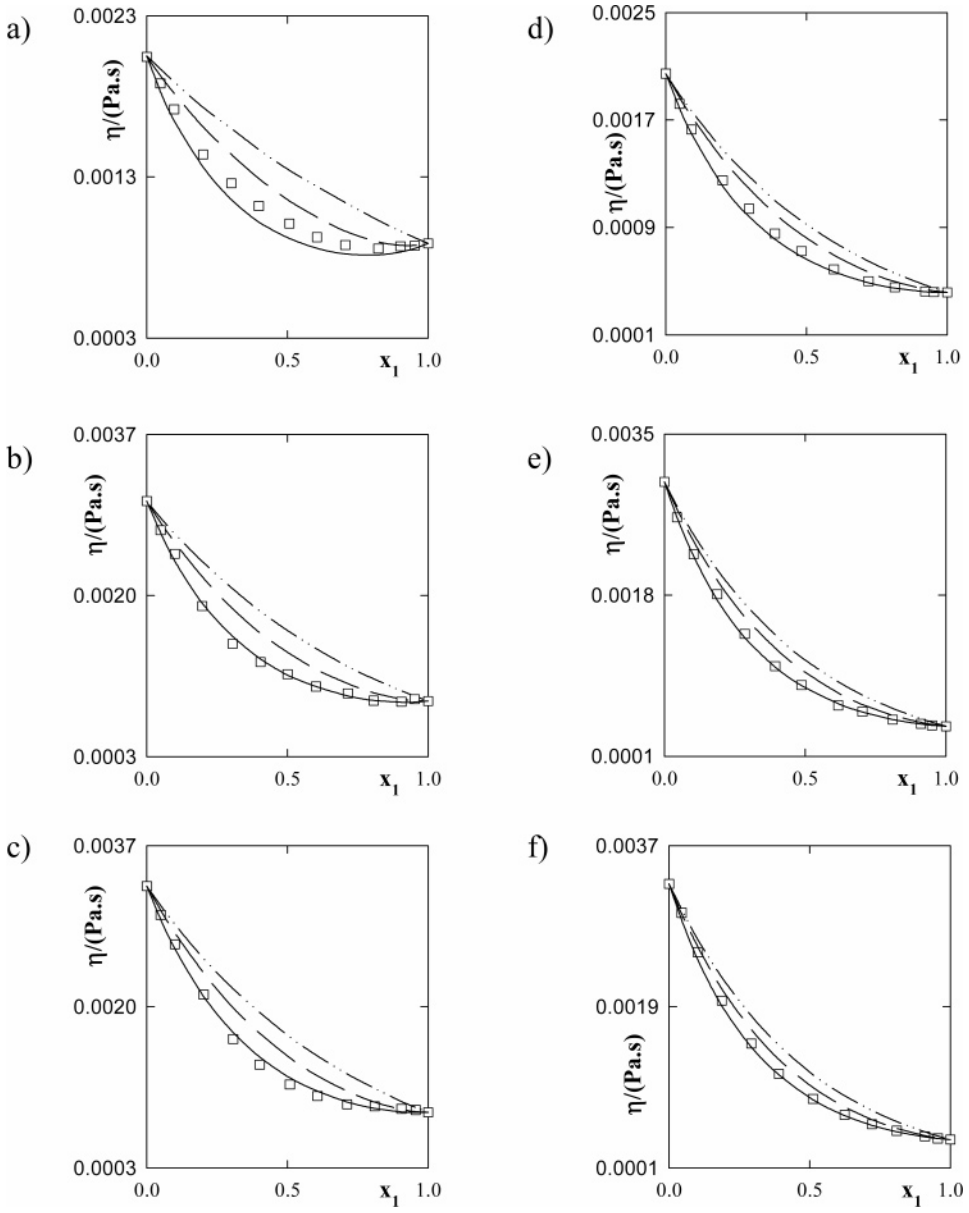

Figure 4. Predicted values of dynamic viscosity, η, from UNIFAC−VISCO (−) using Chevalier parameters, UNIFAC−VISCO (− − −) using new parameters, and ASOG−VISCO (−··−) methods plotted against mole fraction at $T = 298.15$K (□ experimental data) for the binary mixtures (a) cyclohexane (1) + 2-propanol (2) and (b) cyclohexane (1) + 2-butanol (2), (c) cyclohexane (1) + 2-pentanol (2), (d) cyclopentane (1) + 2-propanol (2), (e) cyclopentane (1) + 2-butanol (2), and (f) cyclopentane (1) + 2-pentanol (2).

Table 12. Average Absolute Deviation (AAD) of Dynamic Viscosity Resulting by Predictions Using UNIFAC−VISCO and ASOG−VISCO Methods for Binary Mixtures Cyclohexane (1) and Cyclopentane (1) with 2-Propanol (2), 2-Butanol (2), and 2-Pentanol (2) at Several Temperatures

systems	*T*/K	AAD UNIFAC−VISCO (new parameters)	AAD UNIFAC−VISCO (Chevalier's parameters)	AAD ASOG−VISCO
cyclohexane (1) + 2-propanol (2)	293.15	6	9	21
	298.15	5	8	19
	303.15	6	8	19
cyclohexane (1) + 2-butanol (2)	293.15	2	13	26
	298.15	2	12	24
	303.15	2	11	23
cyclohexane (1)+ 2-pentanol (2)	293.15	4	13	25
	298.15	3	12	23
	303.15	3	11	22
cyclopentane (1) + 2-propanol (2)	293.15	3	11	20
	298.15	3	11	20
	303.15	3	10	19
cyclopentane (1) + 2-butanol (2)	293.15	1	11	22
	298.15	1	10	21
	303.15	2	9	19
cyclopentane (1) + 2-pentanol (2)	293.15	2	8	19
	298.15	2	7	17
	303.15	2	7	17

tively. The fitting parameters (τ_{12}, τ_{21}) together with the objective function (OF) are reported in Table 9.

Figure 3 shows the viscosity data correlated by the UNIQUAC equation for the binary systems cyclohexane (1) and cyclopentane (1) with 2-propanol (2), 2-butanol (2), and 2-pentanol (2). It can be seen that this equation fits the experimental data fairly well at several temperatures.

Prediction using the UNIFAC−VISCO and ASOG−VISCO methods has been performed. The results of the prediction of these systems are not good when we use the interaction parameters of the Chevalier UNIFAC−VISCO method. Then, to improve the results of the prediction of the UNIFAC−VISCO method for the systems cycloalkanes−secondary alcohols, we have determined a new UNIFAC−VISCO interaction parameter $CH_{cy}-OH_s$. The interaction parameters for the CH_2-CH_3, CH_2-CH_{cy}, CH_3-CH_{cy}, CH_2-OH_s, and CH_3-OH_s groups were recalculated in a previous paper.[3,24]

Table 10 shows the experimental data used for calculating new interaction parameters, pointing out the corresponding binary systems employed. These parameters have been determined from experimental values of dynamic viscosity applying the Nelder and Mead[25] equation by minimizing eq 11.

The UNIFAC−VISCO interaction parameters (α_{mn}) are summarized in Table 11. The predictions applying UNIFAC−VISCO using new parameters were compared with the predictions applying UNIFAC−VISCO using Chevalier parameters and ASOG−VISCO methods.

Table 12 shows the average absolute deviation of dynamic viscosity (AAD) resulting from the prediction using UNIFAC−VISCO with Chevalier parameters, UNIFAC−VISCO with the review parameters, and ASOG−VISCO methods for the binary mixtures of cyclohexane (1) and cyclopentane (1) with 2-propanol (2), 2-butanol (2), and 2-pentanol (2) at T = (293.15, 298.15, and 303.15) K.

Figure 4 shows graphs of the experimental dynamic viscosities and the predicted values by applying UNIFAC−VISCO using Chevalier parameters, UNIFAC−VISCO using new parameters, and ASOG−VISCO for all studied systems at T = 298.15 K.

5. Conclusions

In this work, the dynamic viscosities, densities, and speeds of sound of cyclohexane (1) and cyclopentane (1) with 2-propanol (2), 2-butanol (2), and 2-pentanol (2) at several temperatures T = (273.15, 298.15, and 303.15) K over the whole composition range have been determined.

Excess molar volumes, excess molar isentropic compressibilities, and viscosity deviations were calculated and fitted to the Redlich−Kister equation to test the quality of the experimental values. The correlation of the experimental viscosity data has been determined using the UNIQUAC equation. Very good results have been obtained with this equation.

With the experimental data, the interaction parameters of CH_{cy}/OH_S were determined. Using these parameters, the prediction of the dynamic viscosities of the studied systems was calculated. This prediction was compared with the prediction from UNIFAC−VISCO using Chevalier parameters and with ASOG−VISCO methods. We can observe that with ASOG−VISCO method the obtained deviations are higher. Using our new parameters, the UNIFAC−VISCO method better predicts the viscosity of systems with this kind of interaction than using the original UNIFAC−VISCO method.

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