Effect of Composition and Temperature upon Density, Viscosity, Surface Tension, and Refractive Index of 2,2,4-Trimethylpentane + Cyclohexane + Decane Ternary Liquid Systems

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The influence of temperature on the density, viscosity, surface tension, and refractive index of 2,2,4-trimethylpentane (isooctane) + cyclohexane + *n*-decane has been determined at atmospheric pressure. Measurements were made over the temperature range 20 °C to 50 °C. The experimental values of viscosity were correlated with mole fraction of the components using the McAllister and Grumberg−Nissan equations. The experimental data have been used to calculate deviations. The results were fitted to the Redlich−Kister equation.

Introduction

Physical properties are needed in chemical and engineering processes because of their influence upon the effectiveness of the operations. Mass and heat transfer processes and flow operations are evident examples of the importance of the knowledge of these properties.[1,2]

The present work on these properties of the ternary mixtures is a continuation of our recent works[3,4] on the physical properties of the mixtures with the presence of 2,2,4-trimethylpentane and cyclohexane. The system, 2,2,4-trimethylpentane + cyclohexane + decane has not been studied previously while practically all the physical properties for mixtures of "typical" alkanes have been determined.

Densities, viscosities, surface tensions, and refractive indices for the liquid mixtures of isooctane + cyclohexane + decane have been measured over the entire range of compositions at temperatures of 20, 30, 35, 40, 45, and 50 °C. Experimental data of these properties, corresponding to 25 °C, have been published previously.[4] The deviation values for the physical properties for this system have been calculated at these temperatures.

Experimental Section

Materials. All reagents used (2,2,4-trimethylpentane, cyclohexane, and decane) were purchased from Aldrich and Sigma with a stated purity > 99% and used without further purification. Ternary mixtures were prepared by mass using a digital balance (Mettler, model AJ 150, Switzerland), covering the whole composition range of the mixtures. Precautions were taken such as using samples recently prepared and reducing to a minimum the vapor space in the vessels.

In all procedures to determine the value of these physical properties bidistilled water and the pure components employed in the present paper were used to confirm that the methods contributed suitable results using the literature values.[4]

Density Measurements. Densities (ρ) of pure components and their mixtures were obtained using a pycnometric method (Gay−Lussac's pycnometer with a bulb volume of 25 cm^3). The pycnometer containing the mixture was placed in a thermostatic bath maintained constant to ±0.1 °C. Then it was weighed with a Mettler AJ150 balance with a precision of $\pm 10^{-7}$ kg. The uncertainty of the measurement was ± 0.0001 g·cm^{-3}.

Viscosity Measurements. The kinematic viscosity (ν) was determined from the transit time of the liquid meniscus through a capillary viscosimeter supplied by Schott (Cap N° 0c, 0.46 ± 0.01 mm internal diameter, K = 0.003 201 mm^2·s^{-1}) measured with an uncertainty of ±0.000 08 mm^2·s^{-1} using eq 1.

$$\nu = K(t - \theta) \tag{1}$$

where t is the efflux time, K is the characteristic constant of the capillary viscosimeter, and θ is a correction value to prevent the final effects. An electronic stopwatch accurate within ±0.01 s was used for measuring efflux times. The capillary viscometer was immersed in a bath controlled to ±0.1 °C. The viscometer was a Shott-Geräte AVS 350 Ubbelohde viscometer. Each measurement was repeated at least 10 times. The dynamic viscosity (η) was obtained by the product of kinematic viscosity (ν) and the corresponding density (ρ) of the mixture in terms of eq 2 for each temperature and mixture composition.

$$\eta = \rho\nu \tag{2}$$

Surface Tension Measurements. The surface tensions of the mixtures were measured using a Kruss K-9 tensiometer, which employs the Wilhelmy plate principle.[5] The surface tensions of the pure components were determined and compared with literature values to calibrate the tensiometer. The uncertainty of the measurement was ±0.03 mN·m^{-1}. The detailed experimental procedure has been described elsewhere.[6] In general, each surface tension value reported was an average of five measurements. The samples were thermostated in a closed vessel before surface tension measurements to prevent evaporation.

Refractive Index Measurements. Refractive index was determined to within $\pm 1 \times 10^{-6}$ using an Atago RX-1000 refractometer. Before measurements, the refractometer was calibrated using distilled−deionized water in ac-

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Table 1. Densities (ρ), Dynamic Viscosities (η), Surface Tensions (σ), and Refractive Indices (n_D) of Ternary Liquid Mixtures at Several Temperatures

x_1	x_2	ρ/g·cm^{-3}	η/mPa·s	σ/mN·m^{-1}	n_D	x_1	x_2	ρ/g·cm^{-3}	η/mPa·s	σ/mN·m^{-1}	n_D
t = 20 °C											
0.7715	0.1468	0.7019	0.5683	22.2	1.396 85	0.2579	0.5234	0.7356	0.7742	25.3	1.410 81
0.6851	0.1490	0.7127	0.5952	22.2	1.397 99	0.2438	0.6184	0.7333	0.7745	25.3	1.412 44
0.6427	0.2795	0.7068	0.6204	22.6	1.400 17	0.2311	0.7035	0.7501	0.7290	25.4	1.413 94
0.5961	0.1512	0.7125	0.6338	22.6	1.399 08	0.2115	0.1610	0.7255	0.8305	23.7	1.409 46
0.5587	0.2834	0.7099	0.6232	22.7	1.401 58	0.1974	0.3005	0.7300	0.7832	25.4	1.409 60
0.5257	0.4000	0.7156	0.6253	23.2	1.402 79	0.1851	0.4226	0.7210	0.7745	23.9	1.412 50
0.5044	0.1535	0.7149	0.6354	23.4	1.402 22	0.1742	0.5304	0.7415	0.8300	25.6	1.413 36
0.4723	0.2875	0.7205	0.6841	23.5	1.403 50	0.1646	0.6262	0.7240	0.7825	24.1	1.417 00
0.4440	0.4054	0.7364	0.6615	22.9	1.404 40	0.1559	0.7119	0.7495	0.8576	25.7	1.415 40
0.4189	0.5100	0.7165	0.6767	23.6	1.406 10	0.1481	0.7891	0.7445	0.7868	24.0	1.415 50
0.4098	0.1559	0.7227	0.6838	24.3	1.405 49	0.1075	0.1636	0.7284	0.8352	24.3	1.412 50
0.3834	0.2917	0.7223	0.7137	24.4	1.406 80	0.1002	0.3051	0.7345	0.8367	25.9	1.411 30
0.3601	0.4110	0.7439	0.7001	24.5	1.408 04	0.0939	0.4286	0.7427	0.8387	24.3	1.414 60
0.3395	0.5166	0.7300	0.6932	24.6	1.409 50	0.0883	0.5375	0.7440	0.8489	26.2	1.411 22
0.3211	0.6109	0.7360	0.7425	24.6	1.411 11	0.0833	0.6341	0.7562	0.8876	24.5	1.416 18
0.3123	0.1584	0.7122	0.7245	24.5	1.407 26	0.0789	0.7205	0.7510	0.8853	26.4	1.419 50
0.2918	0.2960	0.7272	0.7629	24.9	1.408 18	0.0749	0.7981	0.7372	0.8375	25.1	1.419 62
0.2738	0.4167	0.7398	0.7635	25.1	1.409 47	0.0713	0.8682	0.7286	0.8892	26.7	1.423 90
t = 30 °C											
0.7715	0.1468	0.6936	0.5071	21.1	1.391 95	0.2579	0.5234	0.7265	0.6812	24.0	1.405 79
0.6851	0.1490	0.7034	0.5302	21.5	1.395 30	0.2438	0.6184	0.7246	0.6687	24.2	1.407 19
0.6427	0.2795	0.6982	0.5490	21.3	1.395 18	0.2311	0.7035	0.7472	0.6407	24.3	1.408 82
0.5961	0.1512	0.7030	0.5672	21.5	1.395 33	0.2115	0.1610	0.7172	0.7058	23.2	1.404 42
0.5587	0.2834	0.7023	0.5496	22.2	1.397 39	0.1974	0.3005	0.7215	0.6820	24.3	1.405 46
0.5257	0.4000	0.7097	0.5485	22.6	1.397 47	0.1851	0.4226	0.7135	0.6862	23.2	1.406 21
0.5044	0.1535	0.7069	0.5595	22.6	1.398 55	0.1742	0.5304	0.7322	0.7089	24.5	1.407 37
0.4723	0.2875	0.7110	0.5989	22.7	1.399 68	0.1646	0.6262	0.7169	0.6701	23.1	1.409 54
0.4440	0.4054	0.7273	0.5750	22.4	1.400 50	0.1559	0.7119	0.7395	0.7423	24.6	1.410 08
0.4189	0.5100	0.7089	0.5796	22.6	1.401 99	0.1481	0.7891	0.7366	0.6762	23.0	1.411 03
0.4098	0.1559	0.7148	0.5893	23.2	1.400 82	0.1075	0.1636	0.7204	0.7206	23.4	1.391 95
0.3834	0.2917	0.7157	0.6286	23.3	1.401 98	0.1002	0.3051	0.7265	0.7256	25.0	1.407 27
0.3601	0.4110	0.7354	0.6142	23.2	1.403 04	0.0939	0.4286	0.7343	0.7298	23.6	1.407 40
0.3395	0.5166	0.7223	0.6227	23.4	1.404 30	0.0883	0.5375	0.7352	0.7321	25.0	1.407 43
0.3211	0.6109	0.7282	0.6345	23.3	1.405 77	0.0833	0.6341	0.7516	0.7759	23.6	1.410 53
0.3123	0.1584	0.7047	0.6310	23.9	1.402 67	0.0789	0.7205	0.7432	0.7432	25.4	1.413 08
0.2918	0.2960	0.7183	0.6663	24.0	1.403 53	0.0749	0.7981	0.7293	0.7197	23.6	1.414 23
0.2738	0.4167	0.7304	0.6687	24.0	1.404 57	0.0713	0.8682	0.7207	0.7768	25.4	1.415 03
t = 35 °C											
0.7715	0.1468	0.6903	0.4751	20.5	1.389 44	0.2579	0.5234	0.7241	0.6260	23.5	1.403 09
0.6851	0.1490	0.6993	0.4984	21.1	1.393 77	0.2438	0.6184	0.7211	0.6203	23.7	1.404 69
0.6427	0.2795	0.6937	0.5001	21.0	1.392 46	0.2311	0.7035	0.7432	0.5940	23.7	1.406 06
0.5961	0.1512	0.7020	0.5372	20.8	1.393 36	0.2115	0.1610	0.7121	0.6722	22.3	1.402 75
0.5587	0.2834	0.6977	0.5192	21.4	1.395 31	0.1974	0.3005	0.7185	0.6456	23.8	1.403 07
0.5257	0.4000	0.7058	0.5166	22.0	1.394 44	0.1851	0.4226	0.7098	0.6401	22.4	1.403 78
0.5044	0.1535	0.7024	0.5325	22.0	1.396 72	0.1742	0.5304	0.7295	0.6697	24.0	1.404 75
0.4723	0.2875	0.7075	0.5678	22.2	1.397 74	0.1646	0.6262	0.7130	0.6258	22.5	1.406 75
0.4440	0.4054	0.7224	0.5623	22.1	1.398 46	0.1559	0.7119	0.7355	0.6875	24.0	1.407 34
0.4189	0.5100	0.7056	0.5410	22.2	1.400 00	0.1481	0.7891	0.7318	0.6282	22.4	1.410 50
0.4098	0.1559	0.7111	0.5689	22.6	1.398 50	0.1075	0.1636	0.7158	0.6800	22.8	1.389 44
0.3834	0.2917	0.7115	0.5910	22.8	1.399 57	0.1002	0.3051	0.7230	0.6815	24.4	1.404 88
0.3601	0.4110	0.7316	0.5864	22.8	1.400 56	0.0939	0.4286	0.7292	0.6825	22.9	1.404 80
0.3395	0.5166	0.7200	0.5836	22.8	1.401 58	0.0883	0.5375	0.7320	0.6897	24.4	1.405 05
0.3211	0.6109	0.7247	0.6078	22.8	1.402 74	0.0833	0.6341	0.7471	0.7203	23.0	1.408 75
0.3123	0.1584	0.7013	0.5987	23.4	1.400 27	0.0789	0.7205	0.7394	0.7021	24.8	1.410 45
0.2918	0.2960	0.7160	0.6216	23.4	1.401 11	0.0749	0.7981	0.7248	0.6690	23.1	1.410 62
0.2738	0.4167	0.7258	0.6158	23.6	1.402 15	0.0713	0.8682	0.7164	0.7132	24.8	1.411 52
t = 40 °C											
0.7715	0.1468	0.6850	0.4532	20.2	1.386 80	0.2579	0.5234	0.7190	0.5891	23.0	1.400 79
0.6851	0.1490	0.6955	0.4699	20.4	1.390 39	0.2438	0.6184	0.7175	0.5745	23.0	1.401 64
0.6427	0.2795	0.6901	0.4699	20.7	1.388 80	0.2311	0.7035	0.7385	0.5568	22.9	1.403 01
0.5961	0.1512	0.6908	0.5097	20.4	1.391 91	0.2115	0.1610	0.7086	0.6308	21.7	1.399 56
0.5587	0.2834	0.6933	0.4882	20.8	1.393 30	0.1974	0.3005	0.7112	0.6024	23.2	1.400 72
0.5257	0.4000	0.7014	0.4813	21.5	1.391 85	0.1851	0.4226	0.7055	0.5996	21.8	1.401 22
0.5044	0.1535	0.6980	0.5090	21.4	1.394 96	0.1742	0.5304	0.7220	0.6300	23.4	1.402 27
0.4723	0.2875	0.7015	0.5321	21.5	1.395 80	0.1646	0.6262	0.7083	0.5838	21.9	1.403 21
0.4440	0.4054	0.7186	0.5156	21.5	1.396 42	0.1559	0.7119	0.7280	0.6421	23.4	1.404 50
0.4189	0.5100	0.7015	0.5080	21.6	1.397 81	0.1481	0.7891	0.7279	0.5868	21.9	1.406 23
0.4098	0.1559	0.7062	0.5324	22.1	1.396 18	0.1075	0.1636	0.7153	0.6387	22.2	1.401 12
0.3834	0.2917	0.7045	0.5526	22.1	1.397 18	0.1002	0.3051	0.7185	0.6400	23.9	1.402 54
0.3601	0.4110	0.7266	0.5482	22.2	1.397 98	0.0939	0.4286	0.7259	0.6412	22.3	1.402 00
0.3395	0.5166	0.7120	0.5491	22.3	1.399 06	0.0883	0.5375	0.7251	0.6456	24.0	1.402 75
0.3211	0.6109	0.7195	0.5625	22.3	1.400 06	0.0833	0.6341	0.7420	0.6514	22.5	1.404 52
0.3123	0.1584	0.6966	0.5612	22.8	1.398 10	0.0789	0.7205	0.7312	0.6520	24.2	1.407 32
0.2918	0.2960	0.7085	0.5909	22.9	1.398 73	0.0749	0.7981	0.7209	0.6297	22.7	1.408 02
0.2738	0.4167	0.7213	0.5816	23.1	1.399 65	0.0713	0.8682	0.7127	0.6432	24.2	1.407 85

Table 1. (Continued)

x_1	x_2	ρ/g·cm^{-3}	η/mPa·s	σ/mN·m^{-1}	n_D	x_1	x_2	ρ/g·cm^{-3}	η/mPa·s	σ/mN·m^{-1}	n_D
					t = 45 °C						
0.7715	0.1468	0.6812	0.4287	19.6	1.384 43	0.2579	0.5234	0.7134	0.5656	22.4	1.397 58
0.6851	0.1490	0.6906	0.4459	20.0	1.388 65	0.2438	0.6184	0.7141	0.5389	22.4	1.398 86
0.6427	0.2795	0.6864	0.4474	20.4	1.386 69	0.2311	0.7035	0.7343	0.5245	22.4	1.399 13
0.5961	0.1512	0.6895	0.4780	20.1	1.389 44	0.2115	0.1610	0.7045	0.5995	21.2	1.397 46
0.5587	0.2834	0.6894	0.4679	20.5	1.391 47	0.1974	0.3005	0.7091	0.5621	22.6	1.398 34
0.5257	0.4000	0.6976	0.4596	20.8	1.392 52	0.1851	0.4226	0.7018	0.5696	21.3	1.398 26
0.5044	0.1535	0.6945	0.4885	21.0	1.393 05	0.1742	0.5304	0.7180	0.5824	22.9	1.399 72
0.4723	0.2875	0.6967	0.5044	21.0	1.393 83	0.1646	0.6262	0.7049	0.5530	21.4	1.400 95
0.4440	0.4054	0.7142	0.5000	21.0	1.384 35	0.1559	0.7119	0.7235	0.5978	22.9	1.401 72
0.4189	0.5100	0.6979	0.4806	21.2	1.395 30	0.1481	0.7891	0.7250	0.5547	21.2	1.404 52
0.4098	0.1559	0.7030	0.5104	21.8	1.393 86	0.1075	0.1636	0.7086	0.6010	21.7	1.397 95
0.3834	0.2917	0.7005	0.5231	21.8	1.394 74	0.1002	0.3051	0.7140	0.6015	23.4	1.400 17
0.3601	0.4110	0.7229	0.5123	21.7	1.395 51	0.0939	0.4286	0.7220	0.6020	21.8	1.399 10
0.3395	0.5166	0.7100	0.5182	21.7	1.396 40	0.0883	0.5375	0.7218	0.6030	23.4	1.400 33
0.3211	0.6109	0.7140	0.5314	21.6	1.39 716	0.0833	0.6341	0.7386	0.5987	21.8	1.402 56
0.3123	0.1584	0.6930	0.5297	22.4	1.395 82	0.0789	0.7205	0.7284	0.6030	23.7	1.404 88
0.2918	0.2960	0.7050	0.5595	22.3	1.396 36	0.0749	0.7981	0.7179	0.5874	21.8	1.406 12
0.2738	0.4167	0.7177	0.5488	22.5	1.397 09	0.0713	0.8682	0.7093	0.6010	23.5	1.406 66
					t = 50 °C						
0.7715	0.1468	0.6760	0.3995	19.3	1.382 23	0.2579	0.5234	0.7097	0.5228	21.9	1.394 99
0.6851	0.1490	0.6868	0.4225	19.5	1.386 49	0.2438	0.6184	0.7098	0.5226	21.8	1.396 16
0.6427	0.2795	0.6819	0.4296	19.7	1.384 68	0.2311	0.7035	0.7294	0.4988	21.8	1.396 56
0.5961	0.1512	0.6854	0.4549	19.5	1.387 96	0.2115	0.1610	0.7005	0.5615	20.8	1.395 31
0.5587	0.2834	0.6852	0.4368	19.9	1.391 09	0.1974	0.3005	0.7032	0.5351	22.1	1.396 17
0.5257	0.4000	0.6938	0.4310	20.3	1.390 30	0.1851	0.4226	0.6974	0.5259	20.9	1.395 75
0.5044	0.1535	0.6907	0.4545	20.6	1.391 17	0.1742	0.5304	0.7165	0.5512	22.4	1.397 21
0.4723	0.2875	0.6925	0.4737	20.6	1.391 80	0.1646	0.6262	0.7010	0.5127	20.9	1.398 10
0.4440	0.4054	0.7093	0.4560	20.6	1.392 22	0.1559	0.7119	0.7255	0.5602	22.3	1.398 71
0.4189	0.5100	0.6930	0.4533	20.9	1.393 42	0.1481	0.7891	0.7198	0.5140	20.6	1.402 13
0.4098	0.1559	0.6982	0.4803	21.1	1.391 48	0.1075	0.1636	0.7042	0.5612	21.2	1.394 85
0.3834	0.2917	0.6967	0.4941	21.2	1.392 33	0.1002	0.3051	0.7100	0.5611	22.9	1.397 78
0.3601	0.4110	0.7175	0.4906	21.1	1.392 95	0.0939	0.4286	0.7175	0.5610	21.3	1.397 02
0.3395	0.5166	0.7060	0.4923	21.3	1.392 54	0.0883	0.5375	0.7189	0.5625	22.8	1.397 98
0.3211	0.6109	0.7110	0.5104	21.2	1.393 47	0.0833	0.6341	0.7332	0.5635	21.4	1.399 50
0.3123	0.1584	0.6979	0.5000	21.9	1.393 51	0.0789	0.7205	0.7225	0.5645	23.1	1.402 29
0.2918	0.2960	0.7000	0.5195	21.9	1.394 17	0.0749	0.7981	0.7131	0.5504	21.4	1.402 21
0.2738	0.4167	0.7127	0.5216	22.1	1.394 54	0.0713	0.8682	0.7053	0.5670	22.9	1.403 58

cordance with the instrument instructions. Water was circulated into the instrument through a thermostatically controlled bath maintained constant to ±0.1 °C. The mixtures were directly injected from the stock solution stored at work temperature to avoid evaporation. The refractive index measurements were done after the liquid mixtures attained the constant temperature of the refractometer. This procedure was repeated at least five times. The average of these readings was taken for the refractive index values.

Results and Discussion

Experimental values of densities (ρ), dynamic viscosities (η), surface tensions (σ), and refractive indices (n_D) for 2,2,4-trimethylpentane (1) + cyclohexane (2) + decane (3) ternary mixtures at different temperatures are listed in Table 1. For these ternary systems, Figure 1 shows the density isolines of experimental values at 40 °C. In relation with the effect of temperature, Figure 2 shows the influence of the temperature upon the relation concentration/property value.

The values of excess molar volumes and changes in the physical properties (ΔY) were calculated using the following equations.

$$V^E = \sum_{i=1}^{3} x_i M_i(\rho^{-1} - \rho_i^{-1}) \qquad (3)$$

$$\Delta Y = Y - \sum_{i=1}^{3} x_i Y_i \qquad (4)$$

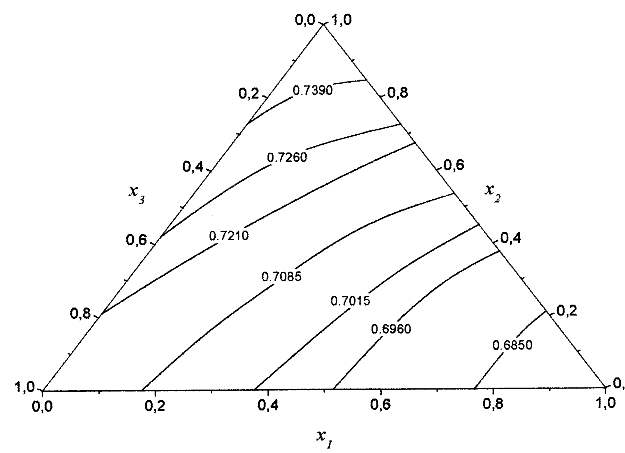

Figure 1. Effect of composition upon the density experimental values at 40 °C.

where x_i, M_i, ρ_i, and Y_i are the molar fractions, molecular weights, densities, and physical properties of the pure components, respectively.

The deviation values were correlated, as a function of composition using the Redlich–Kister equation for ternary systems (eq 5).

$$\Delta Y_{123} = \Delta Y_{12} + \Delta Y_{13} + \Delta Y_{23} + x_1 x_2 x_3 (C_1 + C_2 x_1 + C_3 x_2) \qquad (5)$$

where ΔY_{123} is the deviation considered, x_i is the mole fraction of component i, and ΔY_{ij} is the value of the Redlich–Kister polynomial for the same property fitted to

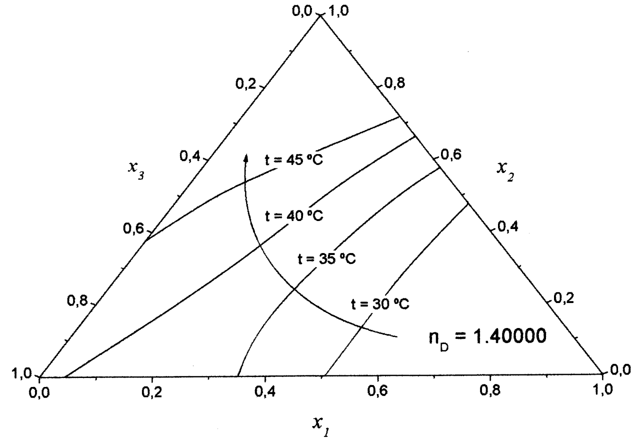

Figure 2. Effect of the temperature on the mixture composition for a fixed value of refractive index.

the data for the corresponding binary system determined by eq 6.[7]

$$\Delta Y = x_1 x_2 \sum_{j=1}^{4} q_j x_2^{(j-1)/2} \tag{6}$$

The calculated parameters corresponding to fit composition/property values to the Redlich−Kister equation are listed in Table 2.

In the case of the viscosity, and according to the literature, the kinematic viscosity/composition values were fitted using the extended McAllister three-body model that is given by the following form:[8]

$$\begin{aligned} \ln \nu = {} & x_1^3 \ln \nu_1 + x_2^3 \ln \nu_2 + x_3^3 \ln \nu_3 + 3x_1^2 x_2 \ln \nu_{12} + \\ & 3x_1^2 x_3 \ln \nu_{13} + 3x_2^2 x_1 \ln \nu_{21} + 3x_2^2 x_3 \ln \nu_{23} + \\ & 3x_3^2 x_1 \ln \nu_{31} + 3x_3^2 x_2 \ln \nu_{32} + 6x_1 x_2 x_3 \ln \nu_{123} - \\ & \ln(x_1 M_1 + x_2 M_2 + x_3 M_3) + x_1^3 \ln M_1 + x_2^3 \ln M_2 + \\ & x_3^3 \ln M_3 + 3x_1^2 x_2 \ln\left[\frac{2M_1 + M_2}{3}\right] + \\ & 3x_1^2 x_3 \ln\left[\frac{2M_1 + M_3}{3}\right] + 3x_2^2 x_1 \ln\left[\frac{2M_2 + M_1}{3}\right] + \\ & 3x_2^2 x_3 \ln\left[\frac{2M_2 + M_3}{3}\right] + 3x_3^2 x_1 \ln\left[\frac{2M_3 + M_1}{3}\right] + \\ & 3x_3^2 x_2 \ln\left[\frac{2M_3 + M_2}{3}\right] + 6x_1 x_2 x_3 \ln\left[\frac{M_1 + M_2 + M_3}{3}\right] \end{aligned} \tag{7}$$

where x_1, x_2, and x_3 are the mole fractions of components 1, 2, and 3 in a ternary mixture, respectively, M_1, M_2, and M_3 are their molecular weights, and ν_1, ν_2, ν_3, and ν are the kinematic viscosities of the pure components and the liquid mixture, respectively. There are six binary parameters ν_{12}, ν_{21}, ν_{13}, ν_{31}, ν_{23}, and ν_{32} and one ternary parameter, ν_{123}. Figure 3 shows the comparison between experimental and calculated values.

The absolute viscosity data were used to test the Grumberg−Nissan model [9] for ternary mixtures. This model had been recommended by different authors[10] for binary mixtures of alkanes.

$$\ln \eta = \sum_{i=1}^{n} x_i \ln \eta_i + \sum_{i=1}^{n} \sum_{j=1}^{n} x_i x_j G_{ij} \qquad i < j \tag{8}$$

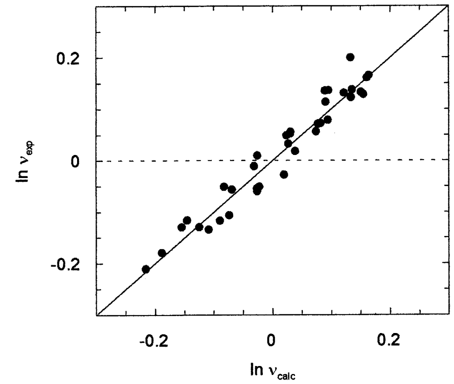

Figure 3. Experimental vs calculated kinematic viscosity values using the McAllister multibody model. t = 20 °C.

Table 2. Coefficients of the Redlich−Kister Type Equation and Root-Mean-Square Deviations (δ)

	20 °C	30 °C	35 °C	40 °C	45 °C	50 °C
			V^E/cm^{-3}·mol^{-1}			
C_1	27.69	24.32	18.21	26.22	29.15	16.62
C_2	−30.47	−1.31	6.75	2.20	1.19	23.53
C_3	−28.28	8.99	9.45	7.37	−2.19	−1.32
δ	0.849	0.868	0.861	0.769	0.753	0.712
			$\Delta\eta$/mPa·s			
C_1	4.41	3.62	3.79	2.97	2.56	1.39
C_2	−2.68	−3.19	−3.26	−2.29	−1.36	−0.20
C_3	−5.99	−3.87	−4.29	−3.61	−3.74	−2.33
δ	0.026	0.021	0.019	0.015	0.013	0.013
			$\Delta\sigma$/mN·m^{-1}			
C_1	−23.5	−36.5	−18.7	−22.2	−22.4	−38
C_2	121.3	130	130.9	141.9	151.5	160.3
C_3	108.4	112.4	105	117.2	90.89	119.2
δ	0.72	0.68	0.71	0.76	0.69	0.69
			Δn_D			
C_1	−0.5126	0.1233	0.1997	0.098	0.1221	−0.0007
C_2	0.2864	−0.1107	−0.1808	−0.0239	−0.1032	0.1004
C_3	0.1513	−0.2342	−0.3512	−0.2719	−0.2504	−0.12
δ	0.0018	0.0008	0.0017	0.0013	0.0019	0.0012

Table 3. Values of the McAllister Three-Body Model and Grumberg−Nissan Model Parameters and Root-Mean-Square Deviations (δ)

	value at the following temperatures					
parameter	20 °C	30 °C	35 °C	40 °C	45 °C	50 °C
			McAllister Parameters			
$10^6\nu_{12}$/m^2·s^{-1}	0.9465	0.7979	0.7462	0.6731	0.6496	0.6344
$10^6\nu_{21}$/m^2·s^{-1}	0.7074	0.6985	0.6666	0.6781	0.6267	0.5517
$10^6\nu_{13}$/m^2·s^{-1}	0.8514	0.7453	0.7045	0.6655	0.6404	0.6704
$10^6\nu_{31}$/m^2·s^{-1}	1.5373	1.2384	1.1364	1.0171	0.9017	0.7624
$10^6\nu_{23}$/m^2·s^{-1}	1.3367	0.9624	0.9623	0.8405	0.8118	1.0344
$10^6\nu_{32}$/m^2·s^{-1}	0.9909	0.9401	0.8882	0.8740	0.8329	1.0738
$10^6\nu_{123}$/m^2·s^{-1}	0.9310	0.9195	0.8710	0.8655	0.8585	0.6551
δ	0.027	0.028	0.023	0.022	0.022	0.028
			Grumberg−Nissan Parameters			
G_{12}	3.9651	4.2441	4.3806	4.5279	4.6510	4.8255
G_{13}	3.0196	3.2250	3.3438	3.3475	3.5504	3.6056
G_{23}	3.4758	3.7143	3.7927	3.8050	3.9439	4.0712
δ	0.175	0.183	0.186	0.189	0.193	0.199

The adjustable parameters (G_{ij}) are determined by fitting experimental viscosity−composition data. Table 3 shows the fitting parameters corresponding to the McAllister and Grumberg−Nissan models, respectively.

The root-mean-square deviations (δ) were calculated, and the values are presented in the tables corresponding to the adjustable parameters for the different models. These deviations were calculated by means of eq 9.

$$\delta = \left(\frac{\sum_i (z_{\mathrm{exp}} - z_{\mathrm{cal}})^2}{n_{\mathrm{data}}} \right)^{1/2} \tag{9}$$

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