Viscosities, Densities, Surface Tensions, and Refractive Indexes of 2,2,4-Trimethylpentane + Cyclohexane + Decane Ternary Liquid Systems at 298.15 K†

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The densities, viscosities, refractive indexes, and surface tensions of ternary mixtures of 2,2,4-trimethylpentane (isooctane) + cyclohexane + decane at 298.15 K and atmospheric pressure were measured. The experimental values of viscosity were correlated with the mole fractions of the components using the McAllister and Grumberg−Nissan equations. These experimental data have been used to calculate deviations. The results were fitted to the Redlich−Kister equation.

Introduction

Alkanes are an important series of homologous, nonpolar, organic solvents. They have often been used in the study of solute dynamics because their physicochemical properties as a function of chain length are well-known.[1] They are also employed in a large range of chemical processes.[2] For this reason, a considerable amount of experimental studies of physicochemical properties have been published in the last 10 years.[3−6]

The physicochemical properties play an important role in the understanding of several industrial processes. Properties such as viscosity or surface tension are required in many empirical equations for different operations such as mass and heat transfer processes. For example, it is necessary to know the mass transfer coefficient to design gas−liquid contactors. To determine the equations that modelize the mass transfer process requires knowledge of the density, viscosity, and surface tension of the liquid phase.

In the present work the viscosities, densities, refractive indexes, and surface tensions of 2,2,4-trimethylpentane + cyclohexane + decane have been measured at 298.15 K.

Experimental Section

2,2,4-Trimethylpentane, cyclohexane, and decane were purchased from Aldrich and Sigma with a stated purity >99% and used without further purification.

The densities (ρ) of the pure components and their mixtures were obtained using a pycnometric method (Gay-Lussac's pycnometer). Doubly distilled-deionized water was used for calibration. The pycnometer containing the mixtures was placed in a thermostatic bath maintained constant to ±0.05 °C. Then it was weighed with a Mettler AJ150 balance with a precision of $\pm 10^{-7}$ kg. Each density value was the average of at least five measurements. Maximum deviations from the average were always <0.1%.

Table 1. Dynamic Viscosities (η), Densities (ρ), Surface Tensions (σ), and Refractive Indexes (n_D) of Pure Compounds at Different Temperatures

ρ/g·cm^{-3}		η/mPa·s		n_D		σ/mN·m^{-1}	
exp	lit.	exp	lit.	exp	lit.	exp	lit.
2,2,4-Trimethylpentane							
0.6860	0.6878[a]	0.4784	0.4620[b]	1.388 58	1.3890[d]	18.60	18.32[e]
	0.6885[b]		0.4780[c]		1.3892[b]		
Cyclohexane							
0.7711	0.7712[f]	0.8958	0.8923[h]	1.422 41	1.4235[i]	24.92	24.65[j]
	0.7737[g]		0.8770[g]		1.4232[g]		
Decane							
0.7267	0.7262[k]	0.8542	0.8590[k]	1.410 14	1.4125[k]	23.95	23.83

[a] TRC d-1490, 1998.[15] [b] Aralaguppi et al., 1999.[16] [c] Aralaguppi et al., 1994.[17] [d] TRC fa-1490, 1998.[15] [e] TRC e-1490, 1998.[15] [f] TRC d-2050, 1998.[15] [g] Aminabhavi et al., 1996.[12] [h] TRC c-2100, 1998.[15] [i] TRC fa-2050, 1998.[15] [j] TRC e-1960, 1998.[15] [k] Lal et al., 2000.[17]

The uncertainty of these measurements was ±0.004 g·cm^{-3}. The measured values for pure components were compared with those existing in the literature (see Table 1).

The kinematic viscosity (ν) was determined from the transit time of the liquid meniscus through a capillary viscometer (0.46 mm of diameter), measured with a precision of ±0.0001 mPa·s (Shott-Geräte AVS 350 Ubbelohde viscometer). An electronic stopwatch accurate within ±0.01 s was used for measuring efflux times. The capillary viscometer was immersed in a bath controlled to ±0.05 °C. The viscometer was calibrated with distilled−deionized water, as recommended by Marsh.[7] The deviations were less than ±0.1%. Each measurement was repeated at least 10 times. The dynamic viscosity (η) was obtained from eq 1.

$$\eta = \rho\nu \tag{1}$$

The surface tensions of the aqueous solutions were measured using a Kruss K-9 tensiometer, which employs the Wilhelmy plate principle.[8] The surface tension of the pure water was determined and compared with literature to calibrate the tensiometer. The detailed experimental procedure has been described elsewhere.[9] The mixtures

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† The present paper forms part of our program on the measurement of physicochemical properties of liquid mixtures.
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Table 2. Dynamic Viscosities (η), Densities (ρ), Surface Tensions (σ), Refractive Indexes (n_D), Excess Molar Volumes (V^E), and Changes on Mixing ($\Delta\eta$, $\Delta\sigma$, Δn_D) of Liquid Ternary Mixtures at 298.15 K

x_1	x_2	ρ/g·cm^{-3}	η/mPa·s	n_D	σ/mN·m^{-1}	V^E/cm^3·mol^{-1}	$\Delta\eta$/mPa·s	Δn_D	$\Delta\sigma$/mN·m^{-1}
0.7682	0.1505	0.6975	0.5564	1.39458	20.76	0.3530	−0.0165	−0.0008	0.9507
0.6891	0.2219	0.7030	0.5715	1.39672	21.20	0.2423	−0.0344	−0.0012	0.8835
0.6822	0.1527	0.7024	0.5925	1.39691	21.80	0.1351	−0.0135	−0.0003	1.4165
0.6740	0.1192	0.7032	0.5976	1.39701	21.55	−0.1038	−0.0103	0.0000	1.1016
0.6479	0.1692	0.7057	0.5790	1.39726	22.20	−0.1781	−0.0408	−0.0009	1.5915
0.6375	0.2854	0.7072	0.5837	1.39789	21.80	0.1562	−0.0444	−0.0020	1.1566
0.5541	0.2895	0.7114	0.6141	1.39952	22.93	0.1247	−0.0461	−0.0022	1.7282
0.5196	0.4071	0.7138	0.6155	1.40022	22.50	0.6265	−0.0623	−0.0037	1.1032
0.5023	0.1574	0.7088	0.6837	1.40048	22.45	0.5478	0.0086	−0.0007	0.8626
0.4684	0.2936	0.7127	0.6748	1.41136	23.12	0.7264	−0.0184	0.0078	1.3463
0.4412	0.3052	0.7139	0.6882	1.40272	23.50	0.7923	−0.0159	−0.0016	1.5476
0.4388	0.4126	0.7180	0.6669	1.40182	23.85	0.5841	−0.0421	−0.0039	1.9143
0.4127	0.5174	0.7216	0.6227	1.40388	23.20	0.7877	−0.1003	−0.0037	1.1203
0.4081	0.1599	0.7130	0.7073	1.40321	22.89	0.4986	−0.0040	0.0000	0.6760
0.3802	0.2979	0.7148	0.6997	1.40443	23.90	1.1554	−0.0275	−0.0011	1.5365
0.3558	0.4182	0.7216	0.6935	1.40553	24.10	0.6669	−0.0475	−0.0020	1.6130
0.3344	0.5240	0.7259	0.6487	1.40704	24.10	0.7338	−0.1045	−0.0023	1.4976
0.3154	0.6178	0.7313	0.7183	1.40801	23.57	0.5869	−0.0457	−0.0029	0.8734
0.3109	0.1624	0.7175	0.7293	1.40495	23.32	0.4011	−0.0192	−0.0003	0.4533
0.2893	0.3023	0.7213	0.7639	1.40587	23.93	0.6096	0.0017	−0.0016	0.9642
0.2705	0.4240	0.7239	0.7042	1.40705	24.50	1.0403	−0.0697	−0.0024	1.4398
0.2704	0.5220	0.7291	0.7366	1.40783	24.49	0.6831	−0.0411	−0.0029	1.4583
0.2540	0.5308	0.7295	0.7289	1.40835	24.60	0.8195	−0.0554	−0.0028	1.4613
0.2451	0.2450	0.7215	1.012	1.40674	24.46	0.6086	−0.0250	−0.0010	1.1757
0.2394	0.6254	0.7342	0.7451	1.40980	24.19	0.7882	−0.0483	−0.0029	0.9776
0.2264	0.7097	0.7407	0.7328	1.41133	23.62	0.4432	−0.0688	−0.0027	0.3520
0.2106	0.1650	0.7207	0.7714	1.40710	24.32	0.5959	−0.0157	−0.0004	0.7807
0.2002	0.0999	0.7214	0.7937	1.40702	24.20	0.1063	0.0051	0.0001	0.5713
0.1958	0.3068	0.7250	0.7961	1.40777	23.13	0.6892	−0.0020	−0.0018	−0.4613
0.1829	0.4299	0.7287	0.7821	1.40814	24.65	0.8771	−0.0256	−0.0033	1.0043
0.1716	0.5378	0.7355	0.7860	1.40992	24.15	0.4338	−0.0301	−0.0031	0.4653
0.1703	0.5210	0.7330	0.7906	1.40902	24.75	0.8060	−0.0254	−0.0038	1.0473
0.1616	0.6331	0.7382	0.7916	1.41033	24.73	0.7842	−0.0319	−0.0041	1.0026
0.1527	0.7180	0.7488	0.7952	1.41263	24.75	−0.2632	−0.0349	−0.0030	0.9885
0.1447	0.7940	0.7474	0.7863	1.41471	24.51	0.7564	−0.0498	−0.0021	0.7180
0.1398	0.3211	0.7286	0.8086	1.40832	24.70	0.4956	−0.0115	−0.0026	0.7330
0.1070	0.1678	0.7242	0.8258	1.40831	24.80	0.7387	−0.0011	−0.0014	0.5675
0.0994	0.3115	0.7302	0.8339	1.40958	24.02	0.4294	−0.0013	−0.0021	−0.2254
0.0927	0.4360	0.7330	0.8362	1.40993	25.03	0.8280	−0.0062	−0.0035	0.7822
0.0869	0.5450	0.7540	0.8594	1.40973	24.73	−2.3730	0.0106	−0.0052	0.4741
0.0818	0.6411	0.7406	0.8351	1.41252	25.10	1.0925	−0.0193	−0.0037	0.8404
0.0773	0.7265	0.7524	0.8369	1.41572	24.98	−0.2017	−0.0224	−0.0017	0.9081
0.0701	0.1794	0.7294	0.8395	1.40843	25.93	−0.1064	−0.0019	−0.0022	0.6935
0.0695	0.8716	0.7557	0.8336	1.41778	24.79	0.7777	−0.0165	−0.0016	0.5194

were thermostated with a precision of ±0.05 °C. In general, each surface tension value reported was an average of 10 measurements.

Refractive index was measured to within ±0.000 01 in an Artago RX-1000 refractometer. The refractometer was calibrated using distilled−deionized water, in accordance with the instrument instructions. Water was circulated into the instrument through a thermostatically controlled bath maintained constant to ±0.05 °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 in 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

A comparison of bibliographic values and our experimental values for the pure compounds is shown in Table 1.

Densities (ρ), refractive indexes (n_D), dynamic viscosities (η), surface tensions (σ), and their changes on mixing of 2,2,4-trimethylpentane (1) + cyclohexane (2) + decane (3)ternary mixtures at 298.15 K are listed in Table 2. These physical properties for the binary mixtures had been obtained from the literature. The surface tensions and refractive indexes for the binary mixture 2,2,4-trimethylpentane + decane and the surface tensions of the cyclohexane + decane mixture were measured. These experimental data are shown in Table 3.

Table 3. Surface Tensions (σ) and Refractive Indexes (n_D) of Liquid Binary Mixtures at 25 °C

2,2,4-Trimethylpentane (1) + Decane (3)			Cyclohexane (2) + Decane (3)	
x_1	σ/mN·m^{-1}	n_D	x_2	σ/mN·m^{-1}
0.0000	23.95	1.409 70	0.0000	23.95
0.2274	23.03	1.406 13	0.3169	24.27
0.4397	21.97	1.402 20	0.5530	24.54
0.6384	20.91	1.397 62	0.7357	24.77
0.8248	19.92	1.393 15	0.8813	24.95
1.0000	19.00	1.389 02	1.0000	25.10

For the ternary systems, Figure 1 shows the density, viscosity, surface tension, and refractive index isolines.

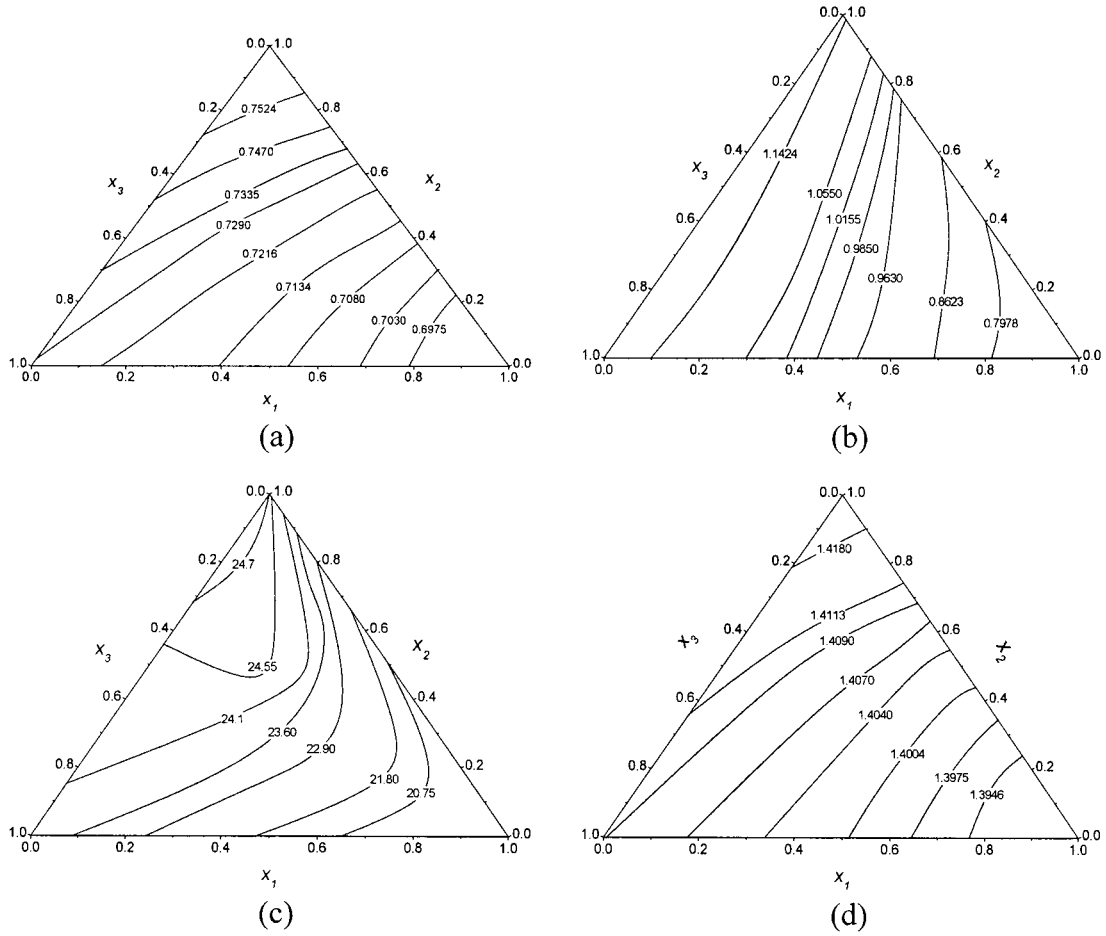

Figure 1. Density (a), dynamic viscosity (b), surface tension (c), and refractive index (d) isolines for 2,2,4-trimethylpentane + cyclohexane + decane ternary mixtures.

Table 4. Values of the McAllister Three-Body Model and Grumberg−Nissan Parameters

McAllister Parameters							
$10^6\nu_{12}/m^2\cdot s^{-1}$	$10^6\nu_{21}/m^2\cdot s^{-1}$	$10^6\nu_{13}/m^2\cdot s^{-1}$	$10^6\nu_{31}/m^2\cdot s^{-1}$	$10^6\nu_{23}/m^2\cdot s^{-1}$	$10^6\nu_{32}/m^2\cdot s^{-1}$	$10^6\nu_{123}/m^2\cdot s^{-1}$	δ
0.7785	0.8681	0.9851	1.0243	1.2445	1.2238	1.0048	0.0187

Grumberg−Nissan Parameters			
G_{12}	G_{13}	G_{23}	δ
4.0664	3.6097	3.4223	0.1781

In the case of the viscosity, and in accordance with the literature, the kinematic viscosity−composition values were fitted using the extended McAllister three-body model, which is given by the following form[10]

$$\begin{aligned}\ln \nu = {} & x_1^3 \ln \nu_1 + x_2^3 \ln \nu_2 + x_3^3 \ln \nu_3 + 3x_1^2x_2 \ln \nu_{12} + \\ & 3x_1^2x_3 \ln \nu_{13} + 3x_2^2x_1 \ln \nu_{21} + 3x_2^2x_3 \ln \nu_{23} + \\ & 3x_3^2x_1 \ln \nu_{31} + 3x_3^2x_2 \ln \nu_{32} + 6x_1x_2x_3 \ln \nu_{123} - \\ & \ln(x_1M_1 + x_2M_2 + x_3M_3) + x_1^3 \ln M_1 + x_2^3 \ln M_2 + \\ & x_3^3 \ln M_3 + 3x_1^2x_2 \ln\left[\frac{2M_1 + M_2}{3}\right] + \\ & 3x_1^2x_3 \ln\left[\frac{2M_1 + M_3}{3}\right] + 3x_2^2x_1 \ln\left[\frac{2M_2 + M_1}{3}\right] + \\ & 3x_2^2x_3 \ln\left[\frac{2M_2 + M_3}{3}\right] + 3x_3^2x_1 \ln\left[\frac{2M_3 + M_1}{3}\right] + \\ & 3x_3^2x_2 \ln\left[\frac{2M_3 + M_2}{3}\right] + 6x_1x_2x_3 \ln\left[\frac{M_1 + M_2 + M_3}{3}\right] \quad (2)\end{aligned}$$

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 2 shows the comparison between experimental and calculated values.

The absolute viscosity data were used to test the Grumberg−Nissan model. This model had been recommended by different authors.[11]

$$\ln \eta = \sum_{i=1}^{n} x_i \ln \eta_i + \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j G_{ij} \qquad i < j \qquad (3)$$

The adjustable parameters, G_{ij}, are determined by fitting experimental viscosity−composition data.

Table 4 shows the fitting parameters corresponding to the McAllister and Grumberg−Nissan models.

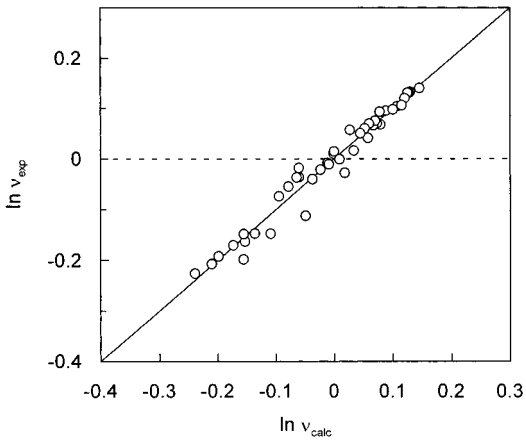

Figure 2. Experimental versus calculated kinematic values using the McAllister equation.

Table 5. Coefficents of the Redlich−Kister Type Equation for the Viscosity Deviation ($\Delta\eta$), Excess Volume (V^E), Surface Tension ($\Delta\sigma$), and Refractive Index Deviation (Δn_D)

property	C_1	C_2	C_3	δ
V^E/cm^{-3}·mol^{-1}	3.8776	12.3968	1.7575	0.5480
$\Delta\eta$/mPa·s	4.2570	−5.5165	−3.0989	0.0230
$\Delta\sigma$/mN·m^{-1}	−50.4119	176.3548	144.3584	0.4200
Δn_D	−0.0066	0.1713	−0.1586	0.0020

For ternary mixtures, the corresponding equation to calculate the changes in the physical properties was defined by eq 4.

$$\Delta Y = Y_m - (x_1Y_1 + x_2Y_2 + x_3Y_3) \quad (4)$$

The deviation values were correlated with the composition data using the Redlich−Kister equation (see Table 5) for ternary systems (eq 5)

$$\Delta Y_{123} = \Delta Y_{12} + \Delta Y_{13} + \Delta Y_{23} + x_1x_2x_3(C_1 + C_2x_1 + C_3x_2) \quad (5)$$

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 the data for the corresponding binary system. When it was possible, ΔY_{ij} of these properties was calculated using data from the literature.[6,12,13] In the case of the surface tensions of 2,2,4-trimethylpentane + decane and cyclohexane + decane, the experimental data were determined. The excess properties were fitted with the Redlich−Kister equation (eq 6).[14]

$$\Delta Y = x_1x_2\sum_{j=1}^{4} q_j x_2^{(j-1)/2} \quad (6)$$

The root-mean-square deviations (δ) had been calculated, and they are presented in the tables. The deviations were calculated by means of eq 7:

$$\delta = \left(\frac{\sum_i (z_{exp} - z_{cal})^2}{n_{data}}\right)^{1/2} \quad (7)$$

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