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Solubility and Density of 2,6-Dimethylnaphthalene in C_1-C_7 1-Alkanols

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Experimental data on the solid−liquid equilibria in 2,6-dimethylnaphthalene (DMN) + C_1-C_7 1-alkanols were obtained over the temperature range of 243.15 K to 343.15 K. The solubility of 2,6-DMN in alcohols increases with increase in polarity of alcohol. The results were well fitted by the best correlation equation. Densities of their binary mixtures have been measured at the temperatures from 253.15 K to 333.15 K and at the mole fractions from 0.0017 to 0.0167. Results for the density were well correlated with the empirical equations.

Introduction

2,6-Dimethylnaphthalene (DMN) is a starting material for the manufacture of polyethylene naphthalate (PEN) and liquid crystal polymer. PEN has especially received much attention because of its higher performance properties in respect to heat resistance, elasticity, chemical stability, and gas barrier than polyethylene terephthalate. Such higher performance properties make it possible to be used in applications such as special films, fibers, reaction containers, and packings.

2,6-DMN must be obtained first to produce PEN. It can be obtained by separation from naphtha oil and by alkylation of naphthalene or xylene.[1,2] These are inevitable for byproduction of DMN isomers, which consist of 10 components. The conventional processes as a distillation and adsorption for separation of 2,6-DMN from the isomer mixtures have a limitation at the purity and yield of products because of isomers.[3] Extractive crystallization was one possibility to apply to separation of multicomponent mixtures.[4,5] A third component, usually a liquid called the extract, induces the change of solid−liquid phase diagram. Findly and Weedman[6] describe in detail an extractive crystallization process in which *p*-xylene and *m*-xylene are completely separated from each other by using *n*-heptane as the extractive solvent. Separation capacity depends mainly on the type of solvent, which affects the kinetic of crystallization such as nucleation and crystal growth. Therefore, selecting the proper solvent is needed before crystallization.

Many organic mixtures with their isomers were separated by extractive crystallization. Solid−liquid-phase equilibria (SLE) must be understood for the possibility of extractive crystallization processes, which in turn are used in the chemical industry for the separation of isomers. The selection of the extractive crystallization process is dependent on the SLE behavior of the mixtures. An extractive solvent to improve the crystal quality must be selected. Alcohols are recommended as a suitable extractive solvent in a cooling crystallizer. The solubility and the density of 2,6-DMN in solution must be known in order to interpret the kinetics of extractive crystallization.

Table 1. Physical Properties of 2,6-DMN and C_1-C_8 Alcohols

compound	T_{fus}/K	T_b/K	ρ/(g cm^{-3})	T_{tri}/K	$\Delta_{fus}H$/(kJ mol^{-1})
2,6-DMN	384.15[7]	535.15[7]	1.020	383.31[7]	25.06[8]
methanol[9]	176.00	337.00	0.786	175.50	2.196
ethanol[9]	159.00	351.50	0.785	158.80	4.962
1-propanol[9]	146.70	370.30	0.799	148.70	5.192
1-butanol[9]	188.00	390.60	0.805	184.50	9.372
1-pentanol[9]	194.60	400.00	0.810	194.20	10.50
1-hexanol[9]	226.00	430.00	0.815	225.80	15.48
1-heptanol[9]	238.60	448.00	0.821	240.00	18.16

In this work, the solubility of 2,6-DMN in C_1-C_7 1-alkanols and densities for their binary mixtures over temperature ranges from 245.15 K to 340.15 K, which is the adequate operating conditions of 2,6-DMN extractive crystallization, have been measured.

Experimental Section

Materials. Reagent-grade 2,6-DMN (Aldrich Chemical Co., +99%) was used. The alcohols used in this work were from Jin Chemical Pharmaceutical Co., reagent-grade with a minimum purity of 99.5%. Before use, 2,6-DMN was purified further by recrystallization using methanol, and the purity was more than 99.9%. All the alcohols were used without further purification. The materials were analyzed by flame-ionization detection gas chromatography (DONAM GC 6200) equipped with capillary columns; Shinwa, GC-8A capillary column ULBON HR-1. The physical properties of 2,6-DMN and C_1-C_8 alcohols are shown in Table 1.

Measurement of Solubility. The mixtures were prepared by mass using a Metter AG 204 balance with a standard uncertainty of 0.0001 g. The estimated accuracy in the mass fraction is less than $\pm 2 \times 10^{-4}$. The solubility of 2,6-DMN in C_1-C_7 1-alkanols was measured using a polythermal method described in detail previously.[10−12] The equilibrium cell, a cylindrical glass vessel (50-mm inside diameter, 120 mm long), was placed, by ground-glass joint, in a triple-jacketed vessel. The outer jacket was evacuated, and either heated or cooled medium from a thermostated bath could be circulated through the middle jacket. A methanol was thermostated and controlled by a thermoelectric Eurotherm 808 PID controller with ±0.1 K accuracy. The cell had a perforated rubber stopper, through

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Table 2. Experimental Solubilities of 2,6-DMN in Various Solvents

methanol		ethanol		1-propanol		1-butanol		1-pentanol		1-hexanol		1-heptanol	
x_1	T/K	x_1	T/K	x_1	T/K	x_1	T/K	x_1	T/K	x_1	T/K	x_1	T/K
0.0074	251.15	0.0057	247.15	0.0045	248.75	0.0040	247.55	0.0044	252.65	0.0030	246.15	0.0015	246.35
0.0097	257.15	0.0119	259.55	0.0096	259.95	0.0084	257.95	0.0075	261.95	0.0107	269.95	0.0043	266.05
0.0175	266.35	0.0188	270.75	0.0165	271.15	0.0142	269.35	0.0152	274.25	0.0216	282.85	0.0097	277.85
0.0232	274.15	0.0314	282.05	0.0258	281.95	0.0266	284.05	0.0255	285.25	0.0315	289.95	0.0187	285.45
0.0330	281.15	0.0414	290.35	0.0469	295.15	0.0384	293.15	0.0418	294.15	0.0426	296.15	0.0302	293.15
0.0470	289.85	0.0523	296.15	0.0601	301.85	0.0543	300.05	0.0507	298.25	0.0600	303.05	0.0421	298.15
0.0712	300.15	0.0736	304.75	0.0699	304.65	0.0637	303.35	0.0750	306.25	0.0713	306.15	0.0605	303.55
0.1064	310.15	0.0806	307.05	0.0783	307.35	0.0781	308.55	0.0832	308.95	0.0868	310.05	0.0764	308.15
0.1285	314.45	0.0907	309.95	0.0928	312.45	0.0990	313.25	0.0943	311.55	0.1011	313.25	0.0921	311.85
0.1588	321.25	0.1058	315.65	0.1050	316.05	0.1176	318.05	0.1121	315.75	0.1205	317.45	0.1149	316.05
0.1808	324.55	0.1268	320.15	0.1155	318.15	0.1372	323.35	0.1447	321.45	0.1490	322.05	0.1390	320.15
0.2044	328.45	0.1535	327.15	0.1418	323.15	0.1557	327.95	0.1808	326.75	0.1915	327.45	0.1615	323.85
0.2388	332.65	0.1884	332.15	0.1818	329.15	0.1834	333.45	0.2152	332.05	0.2228	331.55	0.1806	326.95
0.2639	335.55	0.2096	336.15	0.2037	333.15	0.1930	336.35	0.2651	338.65	0.2464	335.15	0.2081	331.05
												0.2329	333.45
												0.2830	339.05

Table 3. Values of Parameters for Equations 1, 2, and 3 in Various Solvents

system	a/mole fraction	b/(mole fraction K^{-1})	$c \times 10^4$/(mole fraction K^{-2})	$d \times 10^4$/(mole fraction K^{-3})	RSD	AAD
methanol	−7.8719	0.0898	−3.4366	4.4180	0.050914	0.001099
ethanol	−4.8369	0.0560	−2.1805	2.8558	0.029163	0.001376
1-propanol	−8.0238	0.0908	−3.4374	4.3654	0.066315	0.001563
1-butanol	−0.6483	0.0124	−0.6764	1.1332	0.185056	0.002540
1-pentanol	−6.0792	0.0792	−3.0979	4.0521	0.147034	0.001171
1-hexanol	−9.4468	0.1084	−4.1523	5.3155	0.206937	0.001494
1-heptanol	−6.9230	0.0823	−3.2590	4.3035	0.086619	0.001174

which a copper−constantan thermocouple was inserted. The contents were stirred with a magnetic spin bar. The cell was tightly sealed to protect the system from dust and moisture condensation. Mixtures of solute and solvent were cooled in batch until an abundant amount of crystal was formed and then heated very slowly at less than 0.005 K min^{-1} near the equilibrium temperature. The crystal disappearance temperature, detected visually, was measured with a calibrated thermocouple connected to a recorder (data acquisition system). The thermocouples were calibrated with a calibrated thermometer from Fisher Scientific (No. 15-078-7) with a standard uncertainty of 0.05 K. The accuracy of the thermocouple measurements is believed to be ±0.1 K. Some of the experiments were conducted in triplicate to check the reproducibility. The saturation temperature for a given mixture was reproducible within ±0.1 K.

Measurement of Density. The density of solutions of 2,6-DMN + alcohols has been determined using a digital densimeter (Mettler Toledo, AG) with density measurement packages (No. 210260 and No. 238491), which uses the Archimedes' principle. The method was described in detail in our previous works.[10,11] Before measurement, the densimeter was calibrated and water was distilled at the experimental temperatures. The bath temperature was measured with a calibrated thermocouple and maintained constant to ±0.1 K at the desired temperature.

Results and Discussion

Solubility. The mole fraction solubilities of 2,6-DMN from methanol through heptanol were measured over the temperature range from 243 K to 318 K, and the values are listed in Tables 2 and plotted in Figure 1. The solubilities of 2,6-DMN increase with an increase in the temperature and increase with an increase in the number of carbon atoms in alcohols. This means that the solubility of 2,6-DMN in 1-alkanols increases with decreasing polarity of the solvent. The enhancement in the solubility of 2,6-DMN from methanol through heptanol was due to a decrease in the self-association of these alcohols.

Thus, mole fraction solubility of 2,6-DMN, x_1, with the temperature T was analyzed using the polynomial equation

$$x_1 = a + bT + cT^2 + dT^3 \tag{1}$$

where T is the absolute temperature and a, b, c, and d are parameters. The linear expression describes satisfactorily the temperature dependence of the solubility, within the temperature range studied. Table 3 lists the parameters in eq 1 for C_1−C_7 alcohols.

Temperature dependence on solubility is higher at higher alcohol. Therefore, combination of cooling and extractive

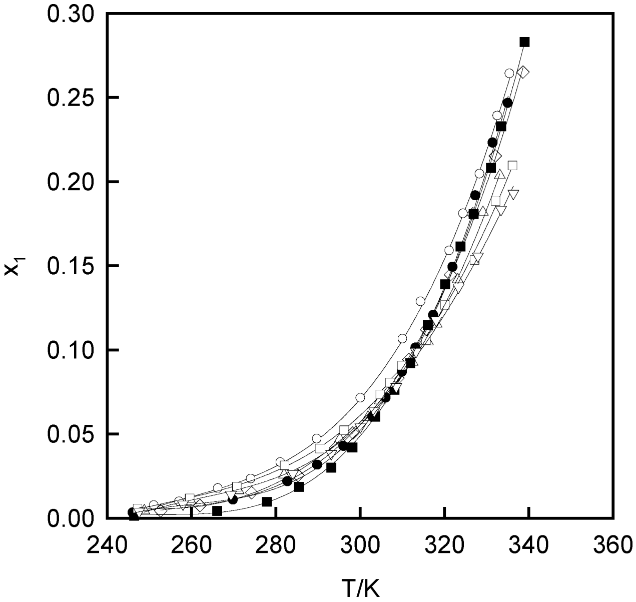

Figure 1. Solubility curves of 2,6-DMN in C_1−C_7 1-alkanol solutions. ○, methanol; □, ethanol; △, 1-propanol; ▽, 1-butanol; ◇, 1-pentanol; ●, 1-hexanol; ■, 1-heptanol.

Table 4. Activity Coefficient of 2,6-DMN in C_1-C_7 1-Alkanols

2,6-DMN(1) + methanol(2)			2,6-DMN(1) + ethanol(2)			2,6-DMN(1) + 1-propanol(2)			2,6-DMN(1) + 1-butanol(2)		
T/K	x_1^L	γ_1^L	T/K	x_1^L	γ_1^L	T/K	x_1^L	γ_1^L	T/K	x_1^L	γ_1^L
253.1500	0.0098	1.7534	253.1500	0.0104	1.6592	253.1500	8.1226×10^{-3}	2.1233	253.1500	0.0102	1.6979
258.1500	0.0122	1.7814	258.1500	0.0126	1.7238	258.1500	0.0100	2.1623	258.1500	0.0123	1.7690
263.1500	0.0151	1.7952	263.1500	0.0153	1.7761	263.1500	0.0124	2.1838	263.1500	0.0148	1.8279
268.1500	0.0187	1.7954	268.1500	0.0185	1.8160	268.1500	0.0153	2.1886	268.1500	0.0179	1.8742
273.1500	0.0231	1.7832	273.1500	0.0224	1.8435	273.1500	0.0189	2.1778	273.1500	0.0216	1.9079
278.1500	0.0286	1.7599	278.1500	0.0270	1.8592	278.1500	0.0234	2.1529	278.1500	0.0261	1.9294
283.1500	0.0353	1.7270	283.1500	0.0327	1.8639	283.1500	0.0288	2.1157	283.1500	0.0314	1.9393
288.1500	0.0434	1.6863	288.1500	0.0394	1.8584	288.1500	0.0354	2.0680	288.1500	0.0378	1.9386
293.1500	0.0534	1.6394	293.1500	0.0475	1.8439	293.1500	0.0435	2.0119	293.1500	0.0454	1.9282
298.1500	0.0655	1.5880	298.1500	0.0571	1.8218	298.1500	0.0534	1.9494	298.1500	0.0545	1.9096
303.1500	0.0801	1.5340	303.1500	0.0685	1.7934	303.1500	0.0653	1.8824	303.1500	0.0652	1.8839
308.1500	0.0976	1.4790	308.1500	0.0820	1.7601	308.1500	0.0797	1.8131	308.1500	0.0779	1.8527
313.1500	0.1185	1.4245	313.1500	0.0980	1.7236	313.1500	0.0968	1.7432	313.1500	0.0929	1.8175
318.1500	0.1431	1.3721	318.1500	0.1165	1.6851	318.1500	0.1173	1.6745	318.1500	0.1103	1.7798
323.1500	0.1719	1.3230	323.1500	0.1381	1.6463	323.1500	0.1414	1.6086	323.1500	0.1306	1.7409
328.1500	0.2050	1.2786	328.1500	0.1630	1.6084	328.1500	0.1694	1.5471	328.1500	0.1540	1.7024
333.1500	0.2427	1.2399	333.1500	0.1913	1.5728	333.1500	0.2018	1.4912	333.1500	0.1806	1.6657

2,6-DMN(1) + 1-pentanol(2)			2,6-DMN(1) + 1-hexanol(2)			2,6-DMN(1) + 1-heptanol(2)		
T/K	x_1^L	γ_1^L	T/K	x_1^L	γ_1^L	T/K	x_1^L	γ_1^L
253.1500	6.7770×10^{-3}	2.5449	253.1500	5.3924×10^{-3}	3.1984	253.1500	5.1613×10^{-3}	3.3416
258.1500	8.5413×10^{-3}	2.5430	258.1500	6.9240×10^{-3}	3.1369	258.1500	6.6356×10^{-3}	3.2732
263.1500	0.0108	2.5200	263.1500	8.8868×10^{-3}	3.0511	263.1500	8.5275×10^{-3}	3.1797
268.1500	0.0135	2.4781	268.1500	0.0114	2.9449	268.1500	0.0110	3.0650
273.1500	0.0170	2.4197	273.1500	0.0146	2.8222	273.1500	0.0141	2.9335
278.1500	0.0214	2.3474	278.1500	0.0187	2.6872	278.1500	0.0180	2.7894
283.1500	0.0269	2.2640	283.1500	0.0239	2.5437	283.1500	0.0231	2.6369
288.1500	0.0337	2.1721	288.1500	0.0306	2.3955	288.1500	0.0295	2.4798
293.1500	0.0422	2.0746	293.1500	0.0390	2.2460	293.1500	0.0377	2.3217
298.1500	0.0527	1.9740	298.1500	0.0496	2.0983	298.1500	0.0480	2.1657
303.1500	0.0656	1.8727	303.1500	0.0629	1.9550	303.1500	0.0610	2.0146
308.1500	0.0815	1.7730	308.1500	0.0794	1.8185	308.1500	0.0772	1.8709
313.1500	0.1007	1.6767	313.1500	0.0999	1.6906	313.1500	0.0972	1.7363
318.1500	0.1238	1.5857	318.1500	0.1249	1.5729	318.1500	0.1218	1.6126
323.1500	0.1514	1.5015	323.1500	0.1550	1.4668	323.1500	0.1515	1.5010
328.1500	0.1839	1.4254	328.1500	0.1909	1.3730	328.1500	0.1869	1.4023
333.1500	0.2215	1.3584	333.1500	0.2328	1.2924	333.1500	0.2284	1.3173

crystallizations can be recommended for separation of 2,6-DMN.

The relative standard deviations (RSD) of the equilibrium temperatures are given by

$$\mathrm{RSD} = \left[\left(\frac{1}{N}\right)\sum_{i=1}^{N}\left[\frac{\mathrm{cal},i - \mathrm{exp},i}{\mathrm{exp},i}\right]^2\right]^{1/2} \qquad (2)$$

and the average absolute deviations (AAD) are given by

$$\mathrm{AAD} = \left(\frac{1}{N}\right)\sum_{i=1}^{N}|\mathrm{cal},i - \mathrm{exp},i| \qquad (3)$$

where N is the number of experimental points. The RSD and the AAD between the measured solubility data and the data calculated from eq 1 are listed in Table 4.

Data of solubility can be used to estimate the activity coefficient through the equilibrium relationship. The following fundamental equation used to calculate the solid−liquid-phase equilibria can be derived starting from the isofugacity criterion.[13] With some useful simplifications it leads to the following formula which was described elsewhere[14]

$$\ln x_1^L\,\gamma_1^L = -\frac{\Delta_{\mathrm{fus}}H_1}{RT}\left(1 - \frac{T}{T_{\mathrm{fus},1}}\right) - \frac{\Delta_{\mathrm{trs}}H_1}{RT}\left(1 - \frac{T}{T_{\mathrm{trs},1}}\right) \qquad (4)$$

where x_1^L is the mole fraction of component 1 (2,6-DMN) in the liquid phase, γ_1^L is the activity coefficient of component 1 in the liquid phase, $\Delta_{\mathrm{fus}}H_1$ is the mole enthalpy of fusion of component 1, $T_{\mathrm{fus},1}$ is the melting temperature of component 1, $\Delta_{\mathrm{trs}}H_1$ is the molar enthalpy of transition of component 1, $T_{\mathrm{trs},1}$ is the transition temperature of component 1, T is the absolute temperature of the mixture, and R is the universal gas constant.

Table 5. Enthalpy of Dissolution and Enthalpy of Mixing for 2,6-DMN in Solvents

solvent	d(ln x_1)/d(T^{-1})	$\Delta_{\mathrm{sol}}H_1$/kJ·mol^{-1}	$\Delta_{\mathrm{mix}}H_1$/kJ·mol^{-1}
methanol	−3562.9	29.6220	4.5620
ethanol	−3314.6	27.5576	2.4976
1-propanol	−3664.9	30.4700	5.4100
1-butanol	−3636.8	30.2364	5.1764
1-pentanol	−4134.9	34.3776	9.3176
1-hexanol	−4196.2	34.8872	9.8272
1-heptanol	−4968.8	41.3106	16.2506

If no solid−solid transition occurs in the considered temperature range, the last term in eq 5 has little effect on the values of the coefficients and has therefore been neglected.[15]

The activity coefficients γ_1^L can be calculated using eq 4 from experimentally determined solution composition x and temperature T. Table 5 gives mole fractions, equilibrium temperatures, and activity coefficients. As can be seen in Table 4, in nearly all the cases, positive deviations from ideal solution ($\gamma_1^L > 1$) are observed. The solubilities of the solute were close to ideal values in the order: methanol < ethanol < propanol < butanol < pentanol < hexanol < heptanol. Such deviations are attributed to the interaction of a chemical nature between the 2,6-DMN and solvent.

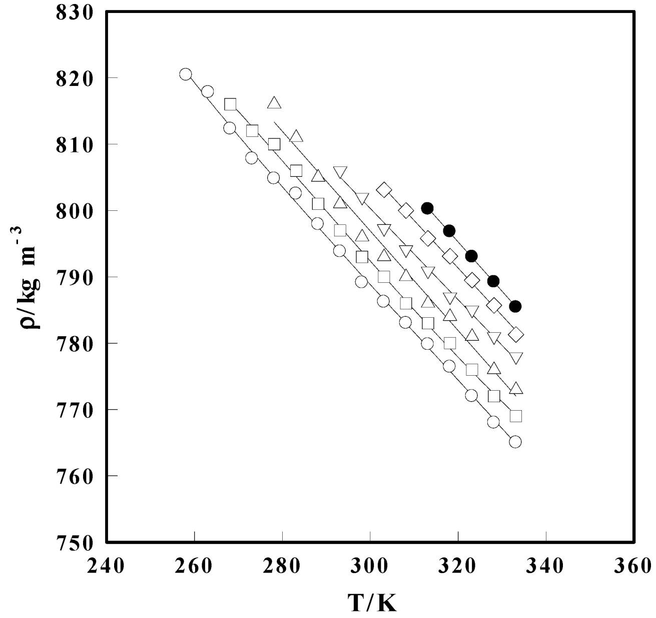

Figure 2. Density of 2,6-DMN + methanol solution at mole fraction: ○, $x = 0.0081$; □, $x = 0.0160$; △, $x = 0.0315$; ▽, $x = 0.0465$; ◇, $x = 0.0610$; ●, $x = 0.0752$.

To procure the enthalpy of dissolution of 2,6-DMN crystals in solvent, mole fraction solubility can be expressed as the following ideal solution theory[10]

$$\ln x_1 = \frac{-\Delta_{\mathrm{sol}}H_1}{R}\left(\frac{1}{T} - \frac{1}{T_{\mathrm{m}}}\right) \tag{5}$$

where x_1 is the mole fraction of solute, $\Delta_{\mathrm{sol}}H_1$ is the enthalpy of dissolution of 2,6-DMN, and T_{m} is the melting temperature of 2,6-DMN. $\Delta_{\mathrm{sol}}H_1$ is equal to $\Delta_{\mathrm{fus}}H_1$ for an ideal system, which is obtained by taking $\gamma_1 = 1$ in eq 4 and $\Delta_{\mathrm{fus}}H_1 + \Delta_{\mathrm{mix}}H_1$ for nonideal systems. The enthalpy of mixing, $\Delta_{\mathrm{mix}}H_1$, is a measure for the solute−solvent interaction, whereas the enthalpy of fusion $\Delta_{\mathrm{fus}}H_1$ is solvent independent. Through the plot of $\ln x_1$ vs T^{-1}, the enthalpy of dissolution was calculated using its slope, $\mathrm{d}\ln x_1/\mathrm{d}T^{-1}$, and its values are listed in Table 5. It was found that $\Delta_{\mathrm{mix}}H_1$ increases with an increase in carbon number in alcohols. This means that attractive interaction between 2,6-DMN and alcohols is larger in alcohol with higher number in carbon atoms. Such a large $\Delta_{\mathrm{mix}}H_1$ shows a large solvent−solute interaction, and this could have a large effect on inclusion of solvent inside crystals.

Density of 2,6-DMN + 1-Alkanols Solution. The densities of 2,6-DMN in 1-alkanol solutions were measured in the range 258.15 K to 333.15 K and mole fraction from 0.0017 to 0.0167. Densities of 2,6-DMN + methanol solution as functions of mole fraction and temperature were shown in Figure 2. Density of solution decreases linearly with increasing temperature. The results of the density for 2,6-DMN + 1-alkanol solutions were correlated for the absolute temperature T and the 2,6-DMN mole fraction x dependence by the following equation

$$\rho = k_1 + k_2x + k_3T + k_4xT \tag{6}$$

where T is the temperature and x is mole fraction of the 2,6-DMN in solutions. The values of coefficients k_1, k_2, k_3, and k_4 of the eq 6 are listed in Table 6 with the AAD, in kgm^{-3}, between the measured value and the calculated value, which is defined in eq 3.

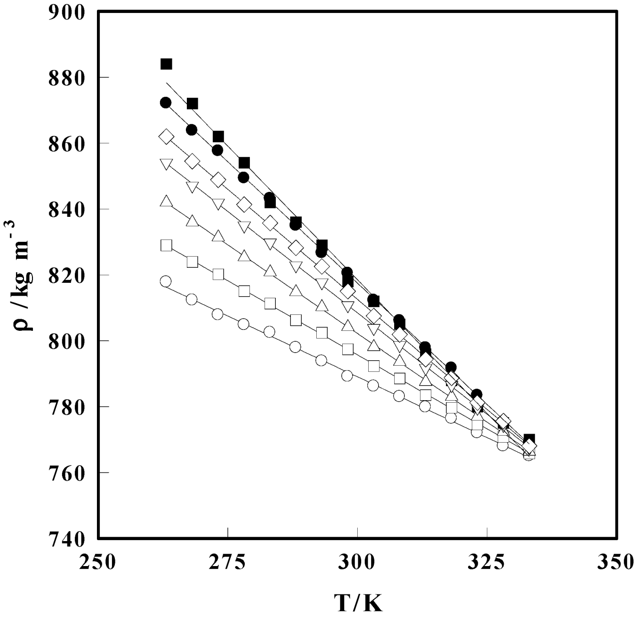

Figure 3. Density of 2,6-DMN + C_1−C_7 1-alkanol solutions at mole fraction $x = 0.0081$. ○, methanol; □, ethanol; △, 1-propanol; ▽, 1-butanol; ◇, 1-pentanol; ●, 1-hexanol; ■, 1-heptanol.

Table 6. Values of Parameters in Equations 3 and 6 for Various Solvents

solvent	k_1	k_2	k_3	k_4	AAD
methanol	501.1243	62889.0062	−0.3691	−45.5671	0.5668
ethanol	533.2065	65716.4937	−0.4496	−55.5094	0.2985
1-propanol	562.9970	69372.4649	−0.5378	−66.4005	0.3571
1-butanol	589.4701	72621.5256	−0.6154	−75.9741	0.4086
1-pentanol	607.3693	74818.2490	−0.6680	−82.4736	0.4436
1-hexanol	628.5796	77875.4051	−0.7365	−90.9196	0.4921
1-heptanol	646.6937	81292.9135	−0.8111	−100.1288	0.9855

Figure 3 shows density of 2,6-DMN + C_1−C_7 1-alkanols at a mole fraction of 0.0081. The density correlation for 2,6-DMN alcohols solution fit the density results with mean deviations of ±0.1%.

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