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A volumetric and viscosity study for the binary mixtures of Benzaldehyde and Pentan-1-ol at 303.15, 308.15, 313.15K and 0.1MPa

K.Saravanakumar[a] and T.R.Kubendran[b]

[a]Department of Chemical Engineering, St.Peter's Engineering College, Avadi, Chennai-600054, India.

[b]Department of Chemical Engineering, A.C. College of Technology, Anna University, Chennai-600025, India.

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ABSTRACT

Densities (ρ) and Viscosities (η) of binary mixtures of Benzaldehyde with Pentan-1-ol have been measured as a function of mole fraction at atmospheric pressure and at different temperatures of (303.15, 308.15and 313.15) K. Using the experimental data, excess volumes (V^E) and deviations in viscosity ($\Delta\eta$) have been calculated. McAllister's three body-interaction model were used to correlate the kinematic viscosity of the systems. The excess volume data was fitted by means of the Redlich-Kister equation. It was found that in all cases the experimental data obtained fitted with the values correlated by the corresponding model very well. The molecular interactions existing between the components were also discussed.

Introduction

The thermodynamic properties of a binary mixture such as viscosity and density are important from practical and theoretical points of view to understand liquid theory. Their properties are extremely useful for the design of process equipment in chemical industries. Binary liquid mixtures due to their unusual behavior have attracted considerable attention [1]. In chemical process industries materials are normally handled in fluid form and as a consequence, the physical, chemical, and transport properties of fluids assume importance. Thus data on some of the properties associated with the liquids and liquid mixtures like Density, viscosity and refractive index find extensive application in solution theory and molecular dynamics [2]. Such results are necessary for interpretation of data obtained from thermo chemical, electrochemical, biochemical and kinetic studies [3]. Benzaldehyde is used chiefly as a precursor to other organic compounds, ranging from pharmaceuticals to plastic additives. It is commonly employed to confer almond flavor. Pentan-1-ol is used as flotation agent and paint manufacturing industry. In the present paper, it has been reported density (ρ) and viscosity (η) of pure benzaldehyde and pentan-ol as well as for the binary system constituted by these two chemicals at temperatures of 303.15, 308.15 and 323.15 K. The viscosity values have been fitted to McAllister [4] model. The deviation values have been fitted to Redlich-Kister type [5] equation. Literature survey showed that no measurements have been previously reported for the mixture studied in this paper.

Expertimental section

Materials

The benzaldehyde of cited purity of 99.5 % and pentan-1-ol with purity of 99.5 % were obtained from Loba chemicals and dried over anhydrous calcium chloride and fractionally distilled before use (6,7).Binary mixtures were gravimetrically prepared with a Shimadzu Corporation Japan type BL 2205 electronic balance with an uncertainty of 0.01 g. Care was taken to avoid evaporation and contamination during mixing. The resulting mole fraction uncertainty was estimated to be less than ±0.0001. All the measurements described below were performed at least three times, and the results presented are the average.

Density

A double- arm pycnometer with a bulb of 25 cm^3 and a capillary of an internal diameter of about 1mm is used to measure the densities (ρ) of pure liquids and binary mixtures. The pycnometer filled with air bubbles free liquids is kept in a thermostat with a thermal stability of ±0.01K for over 30 min to attain thermal equilibrium. The precision of the density measurements was estimated to be ± 0.0003 g ·$cm^{-3.}$

Kinematic Viscosity

The kinematic viscosities were measured with Ostwald viscometer previously calibrated using water. The time was measured with a precision of 0.01 s, and the uncertainty in the viscosity was estimated to be less than 0.0002 mPa·s. The kinematic viscosity was obtained from the working equation

$$v=at-b/t \qquad (1)$$

Where the two constants a and b were obtained by measuring the flow time t of benzene.

Results and discussion

The experimental values of densities (ρ) and viscosities (η) of benzaldehyde with pentan-1-ol and their binary mixtures at various temperatures are listed in Table 1, 2 and 3. Excess molar volumes V^E were calculated from the measured densities (ρ) by using equation

$$V^E=(x_1M_1+x_2M_2)/\rho_m-(x_1M_1/\rho_1+x_2M_2/\rho_2) \qquad (2$$

where ρ_m is the density of the mixture and M_1,ρ_1, x_1 and M_2,ρ_2,x_2 are molecular mass, density and mole fractions of pure benzaldehyde(1) and pentan-1-ol (2), respectively. The uncertainty in the measurement of V^E was found to be ±0.002$cm^3mol^{-1.}$ .The deviations in viscosities, $\Delta\eta$, was computed using the relationship,

Tele:

E-mail addresses: drtrkubendran@yahoo.com, saravanakumarkphd@gmail.com

$\Delta\eta=\eta - (x_1\eta_1 + x_2\eta_2)$ (3)

where η is the dynamic viscosity of the mixture and η_1,x_1 and η_2,x_2 are the viscosity and mole fractions of pure benzaldehyde(1) and pentan-1-ol (2), respectively. The uncertainty in the measurement of $\Delta\eta$ was found to be ±0.001. The viscosities of mixtures of benzaldehyde(1) and pentan-1-ol (2) have been correlated with the model proposed by McAllister [4] for a two-component mixture considering three body interactions.

$$\ln v = x_1^3 \ln v_1 + 3x_1^2 x_2 \ln v_{12} + 3x_1 x_2^2 \ln v_{21} + x_2^3 \ln v_2 - \ln(x_1 + x_2 M_2 / M_1) + 3x_1^2 x_2 \ln((2 + M_2 / M_1)/3) + x_2^3 \ln(M_2 / M_1) + 3x_1 x_2^2 \ln((1 + 2M_2 / M_1)/3) \quad (4)$$

In equation 4, v_1 and v_2 refer to the kinematic viscosity of pure liquids 1 and 2 having mole fractions x_1 and x_2, respectively. The parameters v_{12} and v_{21} represent the interaction parameters obtained by multiple regression analysis, while M_1 and M_2 are the molar mass of the components.

The excess molar volumes and deviations of viscosity were fitted to a Redlich–Kister(5) equation of the type

$$Y = x_1 x_2 \Sigma A_i (x_1 - x_2)^i \quad (5)$$

where Y is either V^E and $\Delta\eta$ and n is the degree of polynomial. Coefficients Ai were obtained by fitting equation 5 to experimental results using a least-squares regression method. In each case, the optimum number of coefficients is ascertained from an examination of the variation in standard deviation (S).S was calculated using the relation

$$S(Y) = [\Sigma(A_{exp} - A_{cal})^2 / (N-n)]^{1/2} \quad (6)$$

Where N is the number of data points and n is the number of coefficients. The calculated values of coefficients along with the standard deviation (S) are given in Table 5 and 6. Interaction parameters and standard deviations of the McAllister model of benzaldehyde(1) and pentan-1-ol (2) mixture at (303.15,308.15 and 313.15) K are presented in Table 4.

Deviation of physical property of liquid mixtures from the ideal behaviour is the measure of the interaction between the molecules which is attributed to either adhesive or cohesive forces.The variation of excess volumes with the mole fraction (X_1) of benzaldehyde(1) and pentan-1-ol at (303.15,308.15 and 313.15)K are represented in figures.1. The excess molar volume values of the mixtures are positive and increase when temperature increases. This shows that the excess molar volumes are always positive for all the studied temperatures. Treszczanowicz et al. (10) and Roux and desnoyers(11) suggested that V^E is the resultant contribution from several opposing effects.

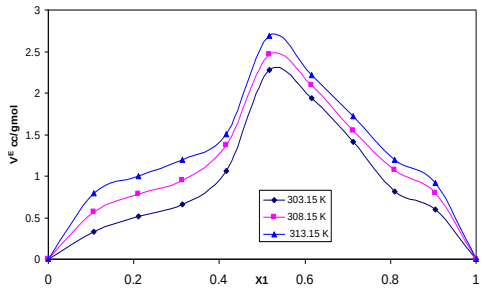

Figure 1: Excess Molar Volume (V^E) for [Benzaldehyde(1)+Pentan-1-ol(2)] :♦ T=303.15 K; ■ T=308.15K; : ▲ 313.15K

In figure 2 Viscosity deviation values were entirely negative (12) for Benzaldehyde-Pentan-1-ol system over, the complete composition range. The physical interactions comprise mainly dispersion forces. Negative deviations occur where dispersion and dipole-dipole forces are operative in the system, but they may also occur, where the components are known to interact more strongly due to chemical and structural fitting of one to another. The deviation increases with increase in temperature. This negative deviation suggests that in these mixtures, the forces between unlike molecules are lesser than the forces between like molecules.

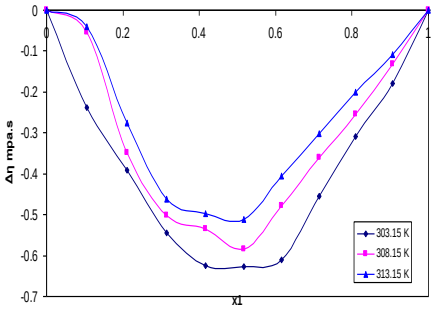

Figure 2: Deviation in viscosity (Δη) for [Benzaldehyde(1)+Pentan-1-ol(2)] :♦ T=303.15 K; ■ T=308.15K; : ▲ 313.15K

Conclusions

Viscosities (η) and Densities (ρ) for the binary liquid mixture of benzaldehyde with penatan-1-ol system was found out as a function of mole fraction at atmospheric pressure and at temperatures of 303.15K, 308.15K, and 313.15K. From the density (ρ) and viscosity (η) data, the values of excess molar volumes (V^E) and the viscosity deviations ($\Delta\eta$) were determined at 303.15K, 308.15K, and 313.15K. Excess molar volumes (V^E) and the viscosity deviations ($\Delta\eta$) were used to predict the intermolecular interactions in the mixtures. McAllister's three-body-interaction model were used to correlate the kinematic viscosity of the systems. The excess volume and viscosity deviation data were fitted by means of the Redlich-kister equation. It was found that in all cases the experimental data obtained, matches with the McAllister model and Redlich-Kister equation with a high degree of precision.

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Table 1: Experimental Densities, dynamic viscosities, viscosity deviations and Excess molar volume for Benzaldehyde (1) + Pentan-1-ol at 303.15 K

X_1	Density(g/cc)	η mpa.s	Δη mpa.s	V^E cc/gmol
0	0.8060	3.0077	0	0
0.1060	0.8266	2.5860	-0.2383	0.3327
0.2105	0.8498	2.2413	-0.3908	0.5165
0.3138	0.8701	1.9200	-0.5449	0.6557
0.4157	0.8891	1.6642	-0.6244	1.0640
0.5163	0.9023	1.4872	-0.6274	2.2822
0.6155	0.9278	1.3337	-0.6093	1.9414
0.7134	0.9552	1.3195	-0.4542	1.4122
0.8101	0.9836	1.2981	-0.3083	0.8146
0.9057	1.0087	1.2628	-0.1782	0.5993
1	1.0378	1.2779	0	0

Table 2: Experimental Densities, dynamic viscosities, viscosity deviations and Excess molar volume for Benzaldehyde (1) + Pentan-1-ol at 308.15 K

X_1	Density(g/cc)	η mpa.s	Δη mpa.s	V^E cc/gmol
0	0.8010	2.6649	0	0
0.1060	0.8198	2.3782	-0.0538	0.5699
0.2105	0.8411	2.0113	-0.3498	0.7789
0.3138	0.8627	1.7107	-0.5013	0.9440
0.4157	0.8821	1.5631	-0.5339	1.3687
0.5163	0.8958	1.3362	-0.5836	2.4594
0.6155	0.9214	1.2983	-0.4783	2.0925
0.7134	0.9488	1.2747	-0.3606	1.5480
0.8101	0.9759	1.2418	-0.2540	1.0755
0.9057	1.0015	1.2252	-0.1326	0.7948
1	1.0324	1.2217	0	0

Table 3: Experimental Densities, dynamic viscosities, viscosity deviations and Excess molar volume for Benzaldehyde (1) + Pentan-1-ol at 313.15 K

X_1	Density(g/cc)	η mpa.s	Δη mpa.s	V^E cc/gmol
0	0.7998	2.385	0	0
0.1060	0.8167	2.2149	-0.0410	0.7988
0.2105	0.8386	1.8518	-0.2768	0.9998
0.3138	0.8592	1.5397	-0.4631	1.1953
0.4157	0.8801	1.3819	-0.4968	1.501
0.5163	0.8922	1.2458	-0.5103	2.6895
0.6155	0.9193	1.2292	-0.4061	2.2135
0.7134	0.9435	1.2150	-0.3010	1.7205
0.8101	0.9741	1.1978	-0.2005	1.1965
0.9057	0.9990	1.1731	-0.1088	0.9141
1	1.0299	1.1670	0	0

Table 4. McAllister interaction parameters and Standard Deviation

Temperature	γ_{12}	γ_{21}	S
303.15K	1.086609	2.034546	1.1114
308.15K	1.091028	1.811992	1.8872
313.15K	1.052716	1.640590	1.23498

Table -5. Redlich Constants and standard deviations

Redlich constants for viscosity deviation							
Temperature	A1	A2	A3	A4	A5	A6	s
303.15K	-2.3667	0.2023	-1.9069	0.4693	4.152	-0.6862	0.05043
308.15K	-2.2128	1.4216	0.7962	-5.6655	1.432	4.2098	0.0466
313.15K	-2.0259	1.6293	1.4636	-6.1381	0.5663	4.4884	0.02501

Table-6. Redlich Constants and standard deviations

Redlich constants for excess volume								
Temperature	A1	A2	A3	A4	A5	A6	A7	s
303.15K	7.8773	7.3184	-29.664	-13.314	72.625	6.1457	-50.824	0.2114
308.15K	8.8025	6.0324	-31.518	-9.9751	88.892	4.0698	-66.163	0.1831
313.15K	9.5923	5.9988	-33.46	-12.589	102.37	6.7145	-78.48	0.2096