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Thermodynamic Properties of Binary and Ternary Mixtures Containing Di-isopropyl Ether, 2-Propanol, and Benzene at $T = 313.15$ K

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Vapor−liquid equilibrium data for the ternary system di-isopropyl ether (DIPE) + 2-propanol + benzene and the binary system 2-propanol + benzene at $T = 313.15$ K are reported. An isothermal total pressure cell has been used for the measurements. Experimental data have been correlated by Barker's method using the Margules equation for the binary system and the Wohl expansion for the ternary system. The Wilson, nonrandom two-liquid (NRTL), and universal quasichemical activity coefficient (UNIQUAC) models have also been applied for the calculations. A comparative study of the effect of the alcohol in mixtures containing DIPE or benzene is included, using the data previously published by the group.

Introduction

Ethers such as isopropyl ether, also known as di-isopropyl ether or DIPE, are potential blending agents in the preparation of the reformulated gasolines. Isopropyl ether is synthesized from reactions between propene and 2-propanol which is also obtained from the hydration of the propene. Therefore, the synthesis of DIPE depends on the availability of propene.

Any process simulation of the synthesis, the purification, or the gasoline blending prior to the design stage needs reliable thermodynamic models for the description of the physical behavior. The highest quality of thermodynamic data is required to improve the interaction parameters of the predictive models which are used in process simulation packages.

Our group is carrying out a research program of the thermodynamic characterization of multicomponent mixtures containing a different type of hydrocarbons (paraffins, cycloparaffins, aromatics, oleffins) and ethers and alcohols as oxygenated additives with the purpose of improving the understanding and the model of the reformulated gasolines.

We performed a series of measurements of ternary mixtures containing DIPE + alcohol + benzene which have been published.[1−4] Now, we report vapor−liquid equilibrium data for the ternary system DIPE + 2-propanol + benzene and the binary system 2-propanol + benzene both at 313.15 K; the other two binary systems involved have been measured previously.[5,6]

Experimental Section

Materials. All of the compounds were purchased from Fluka Chemie AG and were of the highest purity available, chromatography quality reagents (of the series puriss. p.a.) with a stated purity by gas chromatography > 0.990 (GC area) for the DIPE and > 0.995 (GC area) for the benzene and the 2-propanol. They were degassed before measurements by a modified distillation method based on the one suggested by Van Ness and Abbott.[7] The purities of the chemicals were also checked by gas chromatography and were found to be > 0.995 (GC area) for all of the compounds. The average value of the experimental vapor pressures for the pure compounds is compared with those reported in the literature as a check for complete degassing, and the values are summarized in Table 1.

Table 1. Average Values of Experimental Vapor Pressures (p_i^{sat}) for the Pure Compounds Measured in this Work and Literature Values (p_i^{sat}(lit.)), Molar Volumes of Pure Liquids (V_i^{L}), and the Second Virial Coefficients (B_{ii}, B_{ij}) at $T = 313.15$ K Used for the Calculations

	DIPE ($i = 1$)	2-propanol ($i = 2$)	benzene ($i = 3$)
p_i^{sat}/kPa	37.108	13.897	24.386
p_i^{sat}(lit.)/kPa	37.128[a]	13.902[b]	24.398[a]
	37.090[c]	13.853[d]	24.341[e]
	37.081[d]	13.895[f]	24.380[g]
		14.161[e]	
$V_i^{\mathrm{L}}/(\mathrm{cm^3 \cdot mol^{-1}})$[h]	145	78	91
$B_{i1}/(\mathrm{cm^3 \cdot mol^{-1}})$[i]	−1687.8	−1381.9	−1701.0
$B_{i2}/(\mathrm{cm^3 \cdot mol^{-1}})$[i]	−1381.9	−1878.9	−871.0
$B_{i3}/(\mathrm{cm^3 \cdot mol^{-1}})$[i]	−1701.0	−871.0	−1310.5

[a] Ref 6. [b] Ref 5. [c] Ref 24. [d] Ref 25. [e] Ref 22. [f] Ref 26. [g] Ref 27. [h] Ref 28. [i] Calculated by Hayden and O'Connell[15] from Dymond and Smith.[16]

Apparatus and Procedure. A static vapor−liquid equilibrium apparatus, consisting of an isothermal total pressure cell, has been used for measuring the vapor−liquid equilibrium of the binary and ternary mixtures. The apparatus and measuring technique, based on that by Van Ness and co-workers,[8,9] have been described in a previous paper.[10]

Three positive displacement pumps of 100 mL capacity (model: Ruska 2200-801) were used to inject known volumes of degassed components into a cell immersed in a high precision water bath (model: Hart Scientific 6020) assuring a temperature stability of ± 0.5 mK and thermostatted at $T = 313.15$ K. The pump resolution is 0.01 mL, and the resulting uncertainty in the volume injected is ± 0.03 mL.

The cell with a capacity of 180 mL is provided with an externally operated magnetic stirrer. Initially about 50 mL of one component is injected into the evacuated cell, and the vapor pressure is recorded. The second and third components are then injected in appropriate proportions so as to achieve a desired composition. The total mass injected is determined from the

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volume differences corresponding to the initial and final positions of the pistons, the temperature of the injectors, and the densities of the injected component, allowing us assuring an uncertainty in the mole fraction less than $\pm 5 \cdot 10^{-4}$, without sampling the phases.

The temperature was measured by a calibrated standard PRT-100 (model: SDL 5385/100) connected to an alternating current (AC) resistance bridge (model: ASL F250) with a temperature resolution of 1 mK. The estimated uncertainty of the temperature measurement is ± 10 mK. The pressure was measured using a differential pressure cell provided with a null indicator (models: Ruska 2413-705 and 2416-711), respectively. When atmospheric air balances the vapor pressure of the cell, a Bourdon fused quartz precision pressure gauge (model: Texas Instruments 801) provided with a capsule indicates the pressure with an estimated uncertainty of ± 5 Pa for the 125 kPa range. Both temperature and pressure devices have been calibrated with own standards traceable to SI units (International System of Units).

Experimental values of total vapor pressure for the binary mixture were obtained in two overlapping runs starting from opposite ends of the composition range. For the ternary mixture, data were obtained by the addition of a pure species to a mixture of the other two at a fixed temperature. Six runs (dilution lines) were made starting from the corresponding binary system at mole fractions close to 0.3 or 0.7 and adding the third pure component up to a mole fraction of 0.5.

Experimental Results and Correlations

The use of the static measurement technique described above allows a condition of true thermodynamic equilibrium to be established. As a consequence of Duhem's theorem, sampling of the phases is not necessary. Instead, given a set of isothermal pressure and total composition data, thermodynamics allows the calculation of the compositions of the coexisting liquid and vapor phases. Thus, the equilibrium vapor need not be sampled for analysis, and the data are thermodynamically consistent "per se".[11] The data reduction for the binary and ternary mixtures was done by Barker's method[12] according to well-established procedures.[13,14]

The nonideality of the vapor phase was taken into account with the virial equation of state, truncated after the second term. The pure-component and interaction second virial coefficients (B_{ij}) were calculated by the Hayden and O'Connell method[15] using the parameters given by Dymond and Smith,[16] and they are given in Table 1. A correction of the liquid-phase composition has to take into account the vapor space and the very small amount of mass disappearing while evacuating the DPI cell after each point.

The binary system has been correlated by the five-parameter Margules[17] equation:

$$g_{ij} = \frac{G^{\mathrm{E}}}{RT} = \{A_{ji}x_i + A_{ij}x_j - (\lambda_{ji}x_i + \lambda_{ij}x_j)x_ix_j + \eta x_i^2x_j^2\}x_ix_j \tag{1}$$

The three-parameter Wohl equation[18] has been used for the correlation of the ternary system. This model has only three adjustable parameters, C_0, C_1, and C_2, and includes the parameters of the corresponding binaries through the terms g_{ij} given in eq 1.

Table 2. Total Pressure p for the Binary System Benzene (1) + 2-Propanol (2) at $T = 313.15$ K and at Various Compositions of the Liquid Phase x_1 and the Calculated Composition of the Vapor Phase y_1 Using the Five-Parameter Margules Equation

x_1	y_1	p/kPa	x_1	y_1	p/kPa
0.0000	0.0000	13.905	0.5001	0.6636	28.876
0.0594	0.2828	18.356	0.5486	0.6768	29.141
0.0995	0.3826	20.618	0.5501	0.6772	29.140
0.1544	0.4707	23.014	0.5982	0.6898	29.326
0.1954	0.5158	24.383	0.6003	0.6904	29.329
0.2492	0.5594	25.783	0.6499	0.7033	29.455
0.2979	0.5889	26.739	0.7004	0.7166	29.529
0.3484	0.6128	27.503	0.7500	0.7304	29.523
0.3966	0.6315	28.071	0.8149	0.7509	29.381
0.4031	0.6338	28.125	0.8511	0.7655	29.201
0.4478	0.6483	28.525	0.9030	0.7965	28.689
0.4506	0.6492	28.544	0.9468	0.8455	27.679
0.4971	0.6628	28.859	1.0000	1.0000	24.396

$$g_{123} = \frac{G^{\mathrm{E}}}{RT} = g_{12} + g_{13} + g_{23} + (C_0 + C_1x_1 + C_2x_2)x_1x_2x_3 \tag{2}$$

The Wilson,[19] nonrandom two-liquid (NRTL),[20] and universal quasichemical activity coefficient (UNIQUAC)[21] models have also been used for fitting both binary and ternary systems.

The experimental values of total pressure and the mole fractions of the liquid and the vapor phases for the studied systems are given in the Tables 2 and 3. The compositions of the vapor phases are calculated through data reduction.

The data correlation provides the adjustable parameter values of the different models obtained by the method of least-squares. The objective function is defined as the difference between the experimental and the calculated pressures. A Microsoft Excel sheet is programmed with the different models, and the Solver tool is used to obtain the adjustable parameters. The quality of the fitting is analyzed by the root-mean-square of the pressure deviation, the difference between the experimental and the calculated pressures, (rms Δp), and the maximum value of this difference (max $|\Delta p|$).

The results of the correlation are given in Table 4 for the binary system and in Table 5 for the ternary system. Table 6 contains the binary parameters of the Margules equations involved in the Wohl expansion.

Discussion

The binary system measured in this work, benzene + 2-propanol, shows a high positive deviation from the ideality and presents an azeotrope. The best correlation results are obtained for the five-parameter Margules equation, which gives a root-mean-square deviation of pressure of 6 Pa and a maximum value of the deviation of 10 Pa; the Wilson and the NRTL models give higher values but are quite similar between them. The root-mean-square deviations of pressure are (57 and 42) Pa, and the maximum values of the deviations are (154 and 107) Pa, respectively. There are literature data available for comparison, for example, Rhodes et al.,[22] where the reduction of their data using the five-parameter Margules equation gives a root-mean-square of 46 Pa with a maximum deviation of 91 Pa, and the pressure deviations for both data are represented as a function of the liquid composition in Figure 1, which shows the best correlation of our data. The mean deviation between both sets of data is 380 Pa, and there is a difference of 264 Pa on the vapor pressure of the alcohol. As an example, for a composition of 0.75 (which is close to the azeotrope) our experimental pressure is 29.523 kPa, and Rhodes et al. report a

Table 3. Total Pressure p for the Ternary System DIPE (1) + 2-Propanol (2) + Benzene (3) at $T = 313.15$ K and at Various Compositions of the Liquid Phase x_1 and x_2 and the Calculated Vapor Phases y_1 and y_2 Using the Wohl Expansion

x_1	x_2	y_1	y_2	p/kPa
1.0000	0.0000	1.0000	0.0000	37.109
0.7004	0.2996	0.8034	0.1966	37.131
0.6767	0.2895	0.7742	0.1951	36.952
0.6600	0.2823	0.7538	0.1941	36.788
0.6257	0.2676	0.7124	0.1921	36.434
0.5914	0.2529	0.6719	0.1902	36.074
0.5563	0.2379	0.6314	0.1883	35.705
0.5218	0.2231	0.5924	0.1864	35.331
0.4873	0.2083	0.5543	0.1844	34.942
0.4529	0.1936	0.5170	0.1822	34.553
0.4185	0.1789	0.4803	0.1797	34.148
0.3873	0.1655	0.4475	0.1772	33.762
0.3486	0.1490	0.4073	0.1736	33.272
0.0000	1.0000	0.0000	1.0000	13.895
0.3016	0.6984	0.6493	0.3507	30.658
0.2944	0.6815	0.6148	0.3447	30.800
0.2869	0.6642	0.5812	0.3386	30.954
0.2709	0.6268	0.5153	0.3261	31.214
0.2566	0.5937	0.4635	0.3160	31.386
0.2416	0.5588	0.4150	0.3064	31.502
0.2265	0.5239	0.3718	0.2979	31.578
0.2114	0.4888	0.3330	0.2903	31.600
0.1963	0.4539	0.2983	0.2834	31.595
0.1813	0.4190	0.2668	0.2771	31.547
0.1663	0.3844	0.2383	0.2711	31.478
0.1510	0.3490	0.2114	0.2650	31.364
0.0000	0.0000	0.0000	0.0000	24.375
0.3010	0.0000	0.4066	0.0000	29.515
0.2938	0.0240	0.3787	0.0564	30.544
0.2858	0.0505	0.3565	0.1001	31.278
0.2714	0.0984	0.3296	0.1515	32.000
0.2562	0.1490	0.3112	0.1853	32.274
0.2407	0.2004	0.2978	0.2093	32.325
0.2259	0.2497	0.2875	0.2272	32.258
0.2106	0.3003	0.2782	0.2432	32.100
0.1956	0.3503	0.2696	0.2580	31.867
0.1809	0.3992	0.2613	0.2723	31.579
0.1655	0.4504	0.2526	0.2877	31.201
0.1505	0.5000	0.2438	0.3037	30.756
1.0000	0.0000	1.0000	0.0000	37.128
0.7164	0.0000	0.7787	0.0000	34.358
0.6983	0.0253	0.7453	0.0409	34.943
0.6803	0.0504	0.7192	0.0725	35.344
0.6422	0.1035	0.6791	0.1208	35.752
0.6097	0.1489	0.6549	0.1496	35.817
0.5726	0.2008	0.6338	0.1745	35.715
0.5371	0.2503	0.6175	0.1937	35.507
0.5011	0.3006	0.6031	0.2106	35.201
0.4653	0.3505	0.5900	0.2263	34.836
0.4296	0.4003	0.5773	0.2416	34.392
0.3936	0.4506	0.5642	0.2576	33.861
0.3580	0.5002	0.5506	0.2745	33.247
0.0000	1.0000	0.0000	1.0000	13.892
0.0000	0.7020	0.0000	0.4111	26.718
0.0327	0.6790	0.0696	0.3927	27.491
0.0580	0.6612	0.1200	0.3790	28.075
0.0991	0.6323	0.1953	0.3580	28.976
0.1520	0.5951	0.2806	0.3335	30.064
0.2001	0.5613	0.3481	0.3136	30.974
0.2498	0.5264	0.4090	0.2953	31.835
0.2993	0.4916	0.4625	0.2788	32.632
0.3500	0.4561	0.5109	0.2635	33.371
0.4002	0.4208	0.5539	0.2494	34.042
0.4496	0.3861	0.5923	0.2364	34.644
0.4998	0.3509	0.6283	0.2235	35.203
0.0000	0.0000	0.0000	0.0000	24.377
0.0000	0.2996	0.0000	0.2834	29.515
0.0253	0.2920	0.0361	0.2753	29.847
0.0562	0.2828	0.0786	0.2660	30.251
0.1014	0.2692	0.1378	0.2533	30.818
0.1524	0.2539	0.2007	0.2399	31.431
0.1997	0.2397	0.2557	0.2282	31.963
0.2521	0.2240	0.3134	0.2157	32.527
0.3005	0.2095	0.3641	0.2046	33.016
0.3499	0.1947	0.4136	0.1933	33.492
0.4000	0.1797	0.4621	0.1820	33.949
0.4494	0.1649	0.5082	0.1706	34.372
0.4998	0.1498	0.5541	0.1589	34.777

Table 4. Calculated Parameters of the Models Obtained for the Binary System Benzene (1) + 2-Propanol (2) at $T = 313.15$ K, together with the Root-Mean-Square Deviation of Pressure (rms Δp) and the Maximum Value of the Deviation (max $|\Delta p|$)[a]

	Margules	Wilson	NRTL	UNIQUAC
A_{12}	1.4509	0.5469	1.6351	0.6271
A_{21}	2.2095	0.1817	0.8188	0.8901
λ_{12}	0.8271			
λ_{21}	1.9318			
η	1.2685			
α_{12}			0.5634	
rms Δp/kPa	0.006	0.057	0.042	0.207
max $|\Delta p|$/kPa	0.010	0.154	0.107	0.527
$x_{1,\text{azeotrope}}$	0.7227	0.7175	0.7200	0.7071
$p_{\text{azeotrope}}$/kPa	29.536	29.523	29.553	29.474

[a] The Δp term is defined as the difference between the experimental and the calculated pressure.

Table 5. Calculated Parameters of the Models Obtained for the Ternary System DIPE (1) + 2-Propanol (2) + Benzene (3) at $T = 313.15$ K, together with the Root-Mean-Square Deviation of Pressure (rms Δp) and the Maximum Value of the Deviation (max $|\Delta p|$)[a]

	Wilson	NRTL	UNIQUAC	Wohl
A_{12}	0.6747	1.0802	0.3474	$C_0 = 2.9771$
A_{21}	0.3254	0.3924	1.4564	$C_1 = 0.4020$
A_{13}	0.3822	−0.5237	1.1660	$C_2 = -1.0078$
A_{31}	1.6639	0.8434	0.8082	
A_{23}	0.1965	0.8469	1.1436	
A_{32}	0.5300	1.5884	0.4113	
α_{12}		0.4516		
α_{13}		0.3000		
α_{23}		0.5634		
rms Δp/kPa	0.030	0.022	0.047	0.029
max $|\Delta p|$/kPa	0.099	0.048	0.178	0.054

[a] The Δp term is defined as the difference between the experimental and the calculated pressure.

Table 6. Calculated Parameters of the Margules Equation for the Binary Systems Involved in the Ternary System DIPE (1) + 2-Propanol (2) + Benzene (3) at $T = 313.15$ K, Used in the Wohl Expansion

	A_{ij}	A_{ji}	λ_{ij}	λ_{ji}	η
DIPE (i) + 2-propanol (j)[a]	1.0988	1.4201	0.1902	0.4307	
DIPE (i) + benzene (j)[b]	0.2134	0.1277	0.0282	0.0282	
2-propanol (i) + benzene (j)	2.2095	1.4509	1.9318	0.8271	1.2685

[a] Ref 5. [b] Ref 6.

value of 30.175 kPa. Also, we have found a few experimental points of the system at the same conditions report by Storonkin et al.[23] They give lower maximum pressures than those reported by Rhodes et al. A direct comparison of the experimental values is shown in Figure 2, where the total pressure versus the mole fraction of liquid and vapor phases is drawn.

The composition and the pressure of the azeotrope have been calculated using all of the models, and they are given in Table 4. The azeotrope is located at a benzene mole fraction of 0.7227, and the corresponding pressure is 29.536 kPa, using the five-parameter Margules equation.

The high positive deviation from the ideality behavior is also shown with the values of the excess molar Gibbs energy calculated with the Margules equation; a maximum of 1025 J·mol^{-1} is found for a benzene mole fraction of 0.55.

The ternary system DIPE (1) + 2-propanol (2) + benzene (3) has been correlated using the same models and the Wohl expansion. All of the models give similar values of the root-mean-square deviation of the pressure; it ranges from 22 Pa for the NRTL model to 47 Pa for the UNIQUAC model, and the maximum deviations range from (48 to 178) Pa for the same

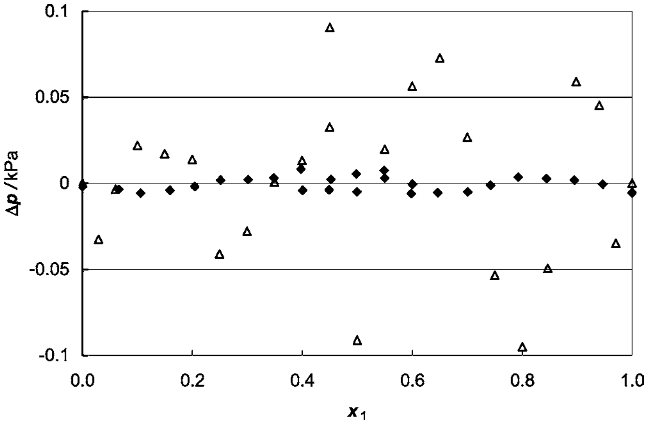

Figure 1. Pressure deviations Δp, defined as differences between experimental and calculated pressures as a function of the liquid composition, x_1, for the system benzene (1) + 2-propanol (2). ◆, this work; △, Rhodes et al.[22]

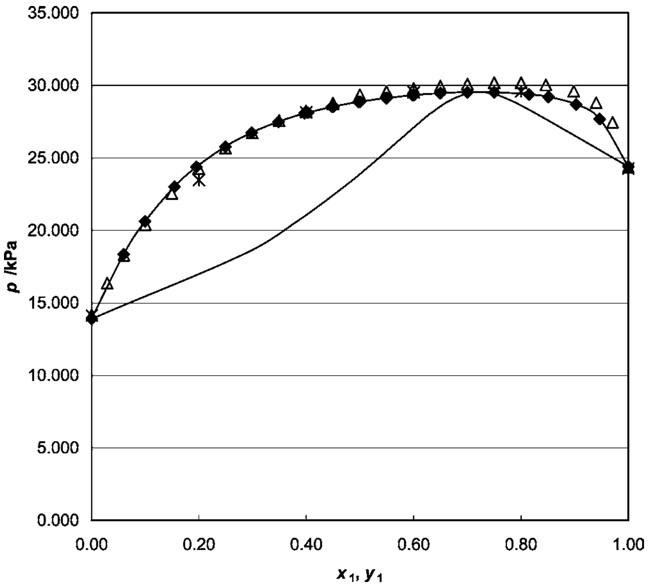

Figure 2. Total pressure at $T = 313.15$ K of the binary system benzene (1) + 2-propanol (2), as a function of the liquid, x_1, and vapor composition, y_1. ◆, this work; △, Rhodes et al.;[22] ∗, Storonkin et al.[23] Symbols represent the experimental points; lines are the calculations of the Margules equation.

models. The ternary pressure surface is shown in Figure 3. In general, the results obtained using the Margules equation and the Wohl expansion are better than the other models, and the Wilson model used to be the best of these semiempirical models.

The experimental values point out that the two azeotropes of maximum pressure, formed in the binary mixtures containing the 2-propanol, disappear when the third component is added to the mixture. The excess molar Gibbs energy was calculated for the ternary system using the Wohl expansion, and the results are presented graphically in Figure 4. It is shown that the highest deviation from the ideality corresponds to the binary system benzene + 2-propanol, as mentioned before.

Finally, a series of ternary systems containing DIPE + benzene + alcohol has been studied, for the alcohols 1-butanol,[4] 2-butanol,[3] isobutanol,[1] 1-propanol,[2] and 2-propanol (presented in this paper). All of the systems show a positive deviation from the ideality. The excess molar Gibbs energies were calculated, and in all of the systems the order of the highest values obtained for the binary systems containing benzene + alcohol was the following: 2-propanol > 1-propanol > isobutanol > 1-butanol > 2-butanol. The maximum values were obtained for a mole fraction of benzene around 0.55. Those values range from (1025 to 885) J·mol^{-1}. Also, those binary mixtures (except for benzene + 1-butanol) exhibit a maximum pressure azeotrope.

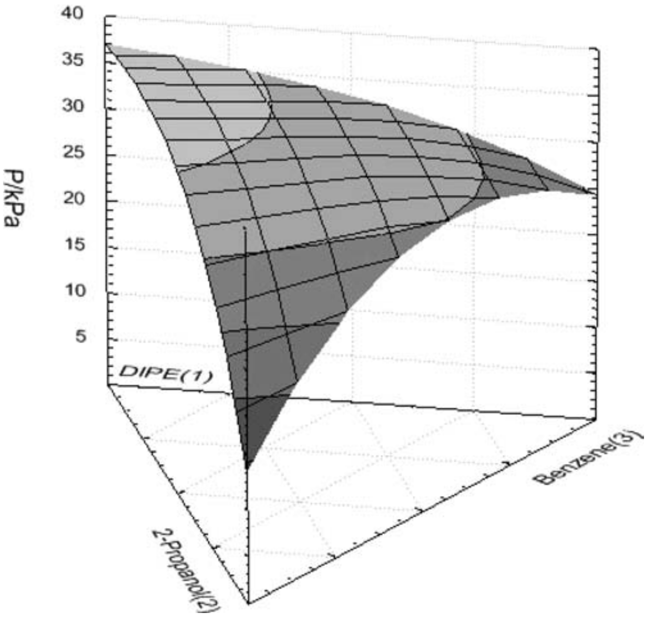

Figure 3. Oblique view of the pressure surface reduced by the Wohl expansion for the ternary system DIPE (1) + 2-propanol (2) + benzene (3) at 313.15 K.

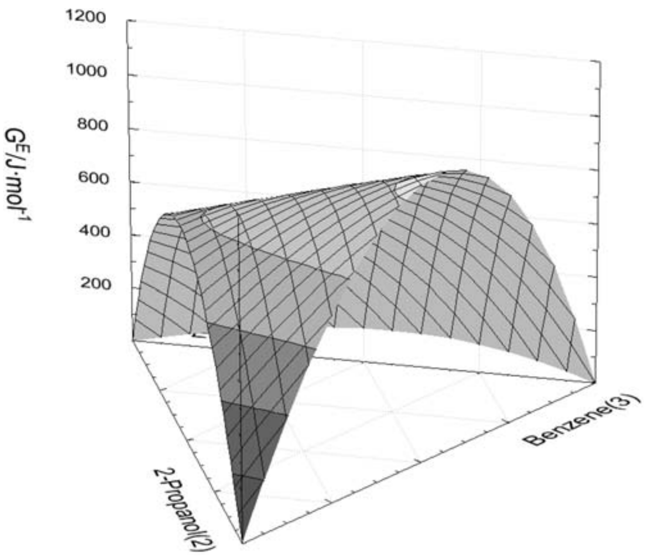

Figure 4. Oblique view of the excess Gibbs energy surface surface reduced by the Wohl expansion for the ternary system DIPE (1) + 2-propanol (2) + benzene (3) at 313.15 K.

The comparison of the binary mixtures DIPE + alcohol give also quite high positive deviations from the ideality whose excess molar Gibbs energies range from (586 to 771) J·mol^{-1} for a mole fraction of the ether around 0.55. The order for the studied alcohols was the following: 2-propanol > 1-propanol > 2-butanol ∼ 1-butanol > isobutanol. Only the system DIPE + 2-propanol shows an azeotrope, and neither of the ternary systems present an azeotrope.

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