Isobaric Vapor–Liquid Equilibria of the Ternary System 1-Pentanol + Nonane + Anisole

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Isobaric vapor–liquid equilibria (VLE) were measured for the ternary system 1-pentanol + nonane + anisole and for two constituent binaries, nonane + anisole and 1-pentanol + anisole, at the pressures (26.66, 53.33, 79.99, and 101.32) kPa. Boiling temperature (T)−liquid composition (x) relations were obtained by using a semimicroebulliometer. A minimum boiling azeotrope was observed in nonane + anisole and in 1-pentanol + anisole. The azeotrope in the ternary system was observed only at the pressure 26.66 kPa. The Wilson equation was used to correlate the binary $T-x$ data and to predict VLE in the ternary system.

Introduction

The thermodynamic information of multicomponent vapor−liquid equilibrium (VLE) is important for testing existing models, for promoting a general understanding of interactions in solutions, and in the design of equipment for separation processes.

In our previous papers,[1–6] we presented experimental results of isobaric vapor–liquid equilibrium (VLE) for ternary systems, where the basic binary mixture was alkane−alcohol. The third components added were compounds with different polarity, *o*-xylene, amyl acetate, methylbutylketone, and dibutyl ether.

Studies of thermodynamic properties of mixtures of alkane−alcohol−ether are of industrial interest. It is known, for example, that anisole can be added to gasoline as a nonmetallic octane number improver. Alcohol−ether is widely used as mixed solvents. These are of interest from a theoretical point of view due to interactions between the ether group and the self-associated primary alcohol.

In the present work, isobaric VLE data have been obtained at pressures of (26.66, 53.33, 79.99, and 101.32) kPa for the ternary system 1-pentanol + nonane + anisole (methyl phenyl ether) and for two constituent binaries containing anisole. No data VLE of the ternary system and the binary nonane + anisole have been found in the literature. Only Orge at al.[7] reported data for 1-pentanol + anisole at 101.32 kPa. We reported VLE data of the binary 1-pentanol + nonane[5,6] and the azeotropic parameters at the pressures (26.66, 53.33, 79.99, and 101.32) kPa. Seymour et al.,[8] Roekens and Verhoeye,[9] and Kushner et al.[10] reported data on the azeotropic parameters for 1-pentanol + nonane at 101.32 kPa.

Experimental Section

Materials. Nonane and 1-pentanol used for the present measurements were the same as those in our early works.[5,6] Anisole was supplied by Fluka.

All substances were fractionally distilled twice in a high-efficiency Teflon spinning band (rotor) column. The samples were collected and stored under argon in glass ampoules. The purity, checked by gas chromatography, was greater than 99.7 % (anisole, 1-pentanol) and 99.8 % (nonane). Densities, refractive indices, and normal boiling temperatures were measured and compared with the literature values in Table 1.

Table 1. Densities ρ, Refractive Indices n_D at 293.15 K, and Normal Boiling Temperatures T_b of Pure Components

	ρ/kg·m^{-3}		n_D		T_b/K	
component	exptl	lit.	exptl	lit.	exptl	lit.
1-pentanol	814.5	814.8[a]	1.4098	1.4100[a]	410.86	410.95[a]
nonane	717.6	717.72[b]	1.4055	1.4054[a]	423.97	423.95[a]
anisole	994.1	994.2[a]	1.5171	1.5170[a]	426.54	426.75[c]

[a] Ref 11. [b] Ref 12. [c] Ref 13.

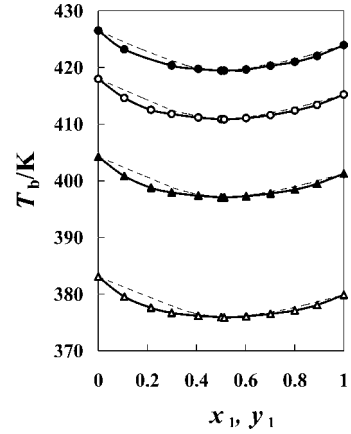

Figure 1. Experimental boiling temperature T_b-x_1 diagrams for nonane (1) + anisole (2) at pressures: Δ, 26.66 kPa; ▲, 53.33 kPa; ○, 79.99 kPa; and ●, 101.32 kPa. Calculated by the Wilson equation[14] curves: solid lines, T_b-x_1; dotted lines, T_b-y_1.

Apparatus and Procedure. The boiling temperature−liquid composition ($T-x$) results were obtained at constant pressure in a semimicroebulliometer with a volume of liquid of about 1 mL. The detail description of the apparatus and procedure has been reported previously.[1] Because the vapor−liquid equilibrium apparatus used in this work was the same as that used in our previous works,[1–6] only a brief description is given here. The

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Table 2. Isobaric Vapor–Liquid Equilibrium Data: Liquid Phase Mole Fraction (x_1) and Boiling Temperatures (T) in Binary Systems

	T/K			
x_1	P = 26.66 kPa	P = 53.33 kPa	P = 79.99 kPa	P = 101.32 kPa
	Nonane (1) + Anisole (2)			
0.000	383.10	404.24	417.99	426.54
0.106	379.56	400.83	414.61	423.19
0.215	377.60	398.80	412.54	–
0.299	376.71	397.96	411.79	420.35
0.407	376.19	397.41	411.18	419.77
0.501	375.94	397.09	410.88	419.46
0.513	375.88	397.08	410.85	419.45
0.602	376.07	397.30	411.08	419.65
0.701	376.52	397.77	411.61	420.31
0.800	377.12	398.47	412.38	420.99
0.891	378.09	399.49	413.41	422.06
1.000	379.88	401.28	415.26	423.97
	1-Pentanol (1) + Anisole (2)			
0.000	383.10	404.24	417.99	426.54
0.127	377.47	397.92	411.46	419.85
0.206	375.58	395.86	409.12	417.38
0.298	374.18	393.92	406.83	414.89
0.386	373.47	392.88	405.48	413.41
0.480	373.00	392.09	404.42	412.15
0.586	372.65	391.36	403.48	411.06
0.691	372.68	391.17	403.13	410.56
0.702	372.70	391.07	403.01	410.40
0.790	372.97	391.13	402.92	410.20
0.900	373.85	391.65	403.10	410.24
1.000	375.63	392.70	403.80	410.86

liquid mixtures were prepared by mass. The equilibrium vessel is connected with a barostat which keeps the pressure at the desired value with the precision of 13 Pa. The boiling temperature of the liquid was measured by a specially manufactured and calibrated thermistor at small different overheating capacities. After the equilibrium was achieved, the resistance of the thermistor was measured and extrapolated into zero overheating capacity. The uncertainties in the boiling temperature, pressure, and liquid mole fraction were estimated to be less than 0.05 K, 13 Pa, and $5 \cdot 10^{-4}$, respectively.

Results and Discussion

The experimental values of boiling temperature measurements for the binary systems nonane + anisole and 1-pentanol + anisole at four pressures, (26.66, 53.33, 79.99, and 101.32) kPa, are reported in Table 2 and presented in Figure 1 and Figure 2.

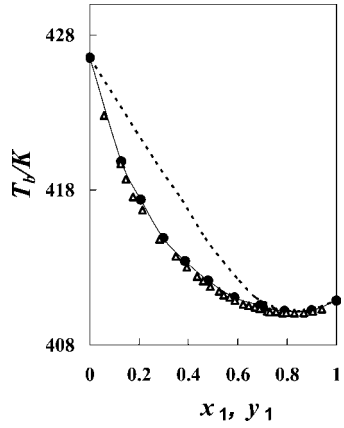

Figure 2. Experimental boiling temperature T_b–x_1 diagram for 1-pentanol (1) + anisole (2) at pressure 101.32 kPa: ●, this work; Δ, from ref 7. Calculated by the Wilson equation[14] curves: solid lines, T_b–x_1; dotted lines, T_b–y_1.

Table 3. Coefficients for the Antoine Equation (Equation 1)

component	A_i	B_i	C_i	temperature region, K
1-pentanol[a]	13.2675	2277.432	−147.537	375 to 415
nonane[b]	13.8546	3224.816	−74.824	375 to 425
anisole	14.2222	3418.456	−70.593	383 to 427

[a] Ref 6. [b] Ref 1.

Table 4. Values of $(\lambda_{ij} - \lambda_{ii})/R$ (the Wilson Equation[14]), Standard Deviations (σP; Equation 3), and Mean Relative Errors (δP; Equation 4) of the Calculated Pressure for Binary Systems

	26.66 kPa	53.33 kPa	79.99 kPa	101.32 kPa
	Nonane (1) + Anisole (2)			
$(\lambda_{12} - \lambda_{11})/R$	955.7	922.7	920.4	834.3
$(\lambda_{21} - \lambda_{22})/R$	1975.0	1864.8	1795.5	1807.5
σP, kPa	0.103	0.173	0.235	0.301
$100\delta P$	0.298	0.224	0.205	0.200
	1-Pentanol (1) + Anisole (2)			
$(\lambda_{12} - \lambda_{11})/R$	1480.3	1130.5	688.3	452.0
$(\lambda_{21} - \lambda_{22})/R$	1943.2	1717.7	1928.9	2069.9
σP, kPa	0.039	0.118	0.170	0.201
$100\delta P$	0.091	0.179	0.154	0.143

Table 5. Azeotropic Boiling Temperatures (T_{az}) and Compositions (x_1^{az}) of the Binary Systems Nonane (1) + Anisole (2) and 1-Pentanol (1) + Anisole (2) vs Pressure (P)

Nonane (1) + Anisole (2)			1-Pentanol (1) + Anisole (2)		
P/kPa	T_{az}/K	x_1^{az}	P/kPa	T_{az}/K	x_1^{az}
26.66	375.9	0.540	26.66	372.6	0.642
53.33	397.1	0.529	53.33	391.1	0.739
79.99	410.8	0.521	79.99	402.9	0.801
101.32	419.4	0.515	101.32	410.2	0.836
–	–	–	101.32	410.05[a]	0.823[a]

[a] Ref 7.

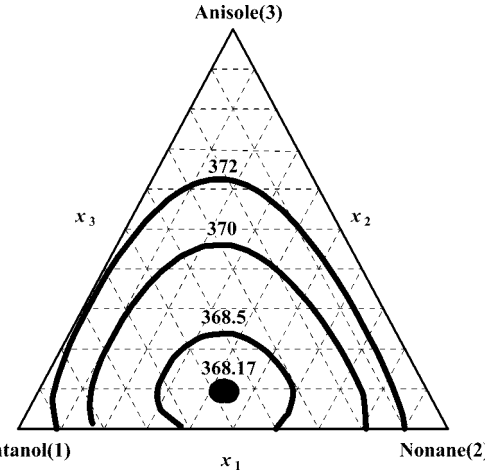

Figure 3. Boiling temperature isotherms, calculated by the Wilson equation,[14] for 1-pentanol (1) + nonane (2) + anisole (3) at 26.66 kPa. The ternary azeotrope is located on the isotherm 368.17 K.

The vapor phase was calculated, considering the ideal behavior of the vapor.

The vapor pressure of pure components P_i^0 was calculated by the Antoine equation

$$\ln(P_i^0/\text{kPa}) = A_i - \frac{B_i}{T/\text{K} + C_i} \quad (1)$$

where A_i, B_i, and C_i and the used temperature regions are reported in Table 3.

Table 6. Experimental Vapor–Liquid Data for the Ternary System 1-Pentanol (1) + Nonane (2) + Anisole (3) at Four Pressures and Values Calculated by the Wilson Equation of Activity Coefficients (γ_1, γ_2, and γ_3), Vapor Mole Fractions (y_1 and y_2), Excess Gibbs Energy (G^E), Pressure (P_{calcd}), Boiling Temperature (T_{calcd}), and Differences in Pressure (ΔP) and Boiling Temperature (ΔT)[a]

experimental data			calculated values									
		T_{exptl}						G^E	P_{calcd}	ΔP	T_{calcd}	ΔT
x_1	x_2	K	γ_1	γ_2	γ_3	y_1	y_2	kJ·mol^{-1}	kPa	kPa	K	K
						$P = 26.66$ kPa						
0.420	0.159	369.88	1.417	2.039	1.195	0.461	0.227	0.335	26.57	−0.09	369.97	0.09
0.319	0.362	368.85	1.635	1.523	1.271	0.386	0.373	0.386	26.54	−0.12	368.96	0.11
0.225	0.549	369.10	2.019	1.250	1.434	0.339	0.467	0.362	26.62	−0.04	369.14	0.04
0.124	0.752	370.48	2.840	1.079	1.772	0.280	0.581	0.258	26.61	−0.05	370.53	0.05
0.714	0.143	369.66	1.102	2.450	1.843	0.598	0.242	0.285	26.82	0.15	369.53	−0.13
0.430	0.285	368.67	1.417	1.726	1.328	0.446	0.330	0.386	26.57	−0.10	368.76	0.09
0.558	0.221	368.70	1.244	1.984	1.491	0.510	0.295	0.361	26.53	−0.14	368.82	0.12
0.461	0.460	368.04	1.436	1.482	1.771	0.472	0.447	0.393	26.52	−0.15	368.17	0.13
0.400	0.400	368.27	1.504	1.507	1.453	0.433	0.398	0.402	26.57	−0.10	368.36	0.09
0.117	0.117	374.58	1.968	2.041	1.020	0.221	0.199	0.178	26.48	−0.19	374.76	0.18
0.606	0.303	368.33	1.205	1.873	1.853	0.526	0.375	0.360	26.59	−0.07	368.39	0.06
0.220	0.110	372.41	1.750	2.095	1.045	0.338	0.179	0.234	26.28	−0.39	372.78	0.37
0.319	0.160	370.62	1.576	1.979	1.110	0.403	0.228	0.309	26.56	−0.11	370.72	0.10
0.509	0.327	368.28	1.318	1.711	1.569	0.482	0.369	0.390	26.62	−0.05	368.32	0.04
0.105	0.597	371.37	2.531	1.182	1.405	0.217	0.514	0.299	27.04	0.38	371.01	−0.36
0.118	0.236	372.81	2.023	1.721	1.060	0.211	0.317	0.249	26.62	−0.04	372.85	0.04
0.297	0.594	368.78	1.870	1.241	1.663	0.404	0.490	0.369	26.91	0.24	368.56	−0.22
0.241	0.278	370.07	1.757	1.654	1.130	0.333	0.327	0.334	26.43	−0.24	370.29	0.22
0.179	0.462	369.85	2.054	1.337	1.261	0.285	0.434	0.346	26.49	−0.17	370.01	0.16
						$P = 53.33$ kPa						
0.420	0.159	389.22	1.346	1.812	1.183	0.495	0.197	0.290	53.33	−0.00	389.22	0.00
0.319	0.362	388.35	1.570	1.409	1.210	0.426	0.341	0.329	53.06	−0.27	388.49	0.14
0.225	0.549	388.88	1.913	1.191	1.317	0.374	0.444	0.304	53.14	−0.20	388.99	0.11
0.124	0.752	390.96	2.537	1.056	1.553	0.296	0.578	0.211	53.13	−0.21	391.07	0.11
0.714	0.143	388.15	1.086	2.328	1.596	0.647	0.218	0.247	53.73	0.40	387.95	−0.20
0.430	0.285	387.93	1.367	1.594	1.260	0.490	0.298	0.333	53.32	−0.02	387.94	0.01
0.558	0.221	387.60	1.210	1.850	1.377	0.556	0.266	0.313	53.24	−0.09	387.65	0.05
0.461	0.460	386.95	1.421	1.398	1.507	0.524	0.408	0.348	53.40	0.07	386.92	−0.03
0.400	0.400	387.41	1.460	1.415	1.331	0.478	0.367	0.348	53.13	−0.20	387.51	0.10
0.117	0.117	395.44	1.949	1.676	1.018	0.251	0.162	0.152	53.75	0.42	395.21	−0.23
0.606	0.303	386.94	1.200	1.762	1.546	0.581	0.338	0.322	53.42	0.09	386.90	− 0.04
0.220	0.110	392.64	1.682	1.741	1.048	0.369	0.146	0.207	53.42	0.09	392.59	− 0.05
0.319	0.160	390.33	1.499	1.717	1.108	0.436	0.195	0.269	53.43	0.10	390.28	−0.05
0.509	0.327	387.18	1.293	1.605	1.403	0.532	0.336	0.341	53.36	0.03	387.16	−0.02
0.105	0.597	392.11	2.358	1.133	1.287	0.240	0.503	0.240	53.95	0.62	391.77	−0.34
0.118	0.236	393.52	1.996	1.492	1.044	0.243	0.277	0.204	53.34	0.01	393.51	−0.01
0.297	0.594	388.12	1.794	1.187	1.471	0.444	0.462	0.318	53.77	0.44	387.89	−0.23
0.241	0.278	390.02	1.689	1.479	1.106	0.370	0.291	0.284	53.00	−0.33	390.20	0.18
0.179	0.462	390.03	1.960	1.249	1.191	0.319	0.408	0.286	53.01	−0.32	390.20	0.17
						$P = 79.99$ kPa						
0.420	0.159	401.81	1.285	1.795	1.150	0.505	0.194	0.257	79.62	−0.38	401.95	0.14
0.319	0.362	401.10	1.492	1.368	1.196	0.436	0.331	0.298	79.32	−0.68	401.36	0.26
0.225	0.549	401.88	1.792	1.161	1.308	0.379	0.436	0.274	79.40	−0.60	402.11	0.23
0.124	0.752	404.51	2.288	1.045	1.516	0.292	0.581	0.187	79.50	−0.50	404.71	0.20
0.714	0.143	400.11	1.079	2.243	1.453	0.673	0.206	0.223	80.28	0.28	400.01	−0.10
0.430	0.285	400.41	1.322	1.544	1.222	0.506	0.287	0.301	79.64	−0.36	400.55	0.14
0.558	0.221	399.84	1.188	1.786	1.300	0.579	0.253	0.282	79.58	−0.42	400.00	0.16
0.461	0.460	399.20	1.399	1.340	1.422	0.549	0.387	0.317	79.76	−0.24	399.29	0.09
0.400	0.400	399.84	1.418	1.364	1.290	0.497	0.351	0.315	79.25	−0.75	400.12	0.28
0.117	0.117	408.86	1.716	1.715	1.019	0.237	0.167	0.140	80.30	0.30	408.74	−0.12
0.606	0.303	399.00	1.193	1.675	1.429	0.610	0.316	0.296	79.86	−0.14	399.05	0.05
0.220	0.110	405.77	1.528	1.775	1.041	0.361	0.150	0.183	79.62	−0.38	405.92	0.15
0.319	0.160	403.18	1.400	1.715	1.092	0.438	0.194	0.239	79.76	−0.24	403.27	0.09
0.509	0.327	399.45	1.272	1.538	1.331	0.556	0.318	0.310	79.76	−0.24	399.54	0.09
0.105	0.597	405.67	2.113	1.112	1.298	0.234	0.499	0.219	80.80	0.80	405.35	−0.32
0.118	0.236	406.98	1.767	1.486	1.051	0.232	0.277	0.193	80.07	0.07	406.95	−0.03
0.297	0.594	400.75	1.718	1.155	1.422	0.457	0.450	0.285	80.06	0.06	400.73	−0.02
0.241	0.278	403.02	1.560	1.454	1.104	0.369	0.287	0.259	79.22	−0.78	403.33	0.31
0.179	0.462	403.21	1.799	1.219	1.200	0.318	0.402	0.262	79.28	−0.72	403.50	0.29
						$P = 101.32$ kPa						
0.420	0.159	409.63	1.303	1.619	1.143	0.527	0.174	0.244	101.04	−0.29	409.72	0.09
0.319	0.362	409.08	1.515	1.322	1.134	0.459	0.319	0.274	100.66	−0.67	409.29	0.21
0.225	0.549	410.05	1.834	1.153	1.178	0.402	0.431	0.251	101.35	0.01	410.05	0.00
0.124	0.752	413.02	2.405	1.046	1.292	0.316	0.576	0.174	102.64	1.30	412.59	−0.43
0.714	0.143	407.56	1.075	2.102	1.464	0.688	0.191	0.212	101.40	0.06	407.54	−0.02
0.430	0.285	408.18	1.329	1.481	1.181	0.525	0.274	0.282	100.83	−0.50	408.34	0.16
0.558	0.221	407.43	1.186	1.705	1.280	0.595	0.240	0.268	100.60	−0.73	407.66	0.23
0.461	0.460	406.78	1.372	1.362	1.298	0.553	0.389	0.308	101.21	−0.12	406.82	0.04

Table 6 Continued

experimental data			calculated values									
		T_{exptl}						G^E	P_{calcd}	ΔP	T_{calcd}	ΔT
x_1	x_2	K	γ_1	γ_2	γ_3	y_1	y_2	kJ·mol^{-1}	kPa	kPa	K	K
					$P = 101.32$ kPa							
0.400	0.400	407.63	1.415	1.352	1.206	0.512	0.346	0.297	100.62	−0.72	407.86	0.23
0.117	0.117	417.30	1.806	1.439	1.013	0.260	0.140	0.122	101.48	0.14	417.25	−0.05
0.606	0.303	406.52	1.175	1.671	1.374	0.617	0.312	0.282	101.13	−0.20	406.58	0.06
0.220	0.110	414.00	1.583	1.507	1.037	0.385	0.126	0.171	101.50	0.17	413.94	−0.06
0.319	0.160	411.19	1.434	1.522	1.083	0.463	0.171	0.224	101.33	0.00	411.19	0.00
0.509	0.327	407.08	1.261	1.521	1.270	0.568	0.312	0.294	101.00	−0.33	407.18	0.10
0.105	0.597	414.20	2.246	1.092	1.168	0.261	0.495	0.184	102.25	0.92	413.89	−0.31
0.118	0.236	415.48	1.868	1.322	1.029	0.258	0.250	0.158	100.57	−0.76	415.74	0.26
0.297	0.594	408.75	1.716	1.168	1.251	0.469	0.449	0.277	102.65	1.31	408.34	−0.41
0.241	0.278	411.15	1.612	1.344	1.071	0.397	0.266	0.230	100.20	−1.13	411.52	0.37
0.179	0.462	411.44	1.873	1.180	1.114	0.345	0.391	0.228	100.30	−1.03	411.78	0.34

[a] Mean relative absolute error (δP) is 0.147 %, and (δT) is 0.055 %.

The $T-x$ data of binary systems were fitted with the Wilson model,[14] writing

$$\ln \gamma_i = -\ln(x_i - \Lambda_{ik}x_k) + x_k\left[\frac{\Lambda_{ik}}{x_i + \Lambda_{ik}x_k} - \frac{\Lambda_{ki}}{x_k + \Lambda_{ki}x_i}\right] \quad (2)$$

where γ_i is the activity coefficient of component i in the liquid phase.

In Table 4, the values of $(\lambda_{ij} - \lambda_{ii})/R$ (the Wilson equation[14]) and standard deviations (eq 3) and mean relative errors (eq 4) for the binaries nonane + anisole and 1-pentanol + anisole are presented.

The standard deviation was calculated using

$$\sigma P = \left[\sum^{N} (P_{calcd} - P_{exptl})^2/(N-n)\right]^{1/2} \quad (3)$$

where P_{calcd} and P_{exptl} are the calculated and experimental values of the total pressure, respectively; N is the number of experimental points; and n is the number of parameters in a correlation model (n is equal to 2). The mean relative error, deviation between experimental and calculated pressure, is defined as

$$\delta P = \frac{1}{N}\sum^{N} |(P_{exptl} - P_{calcd})/P_{exptl}| \quad (4)$$

The azeotropic boiling temperatures (T_{az}) and compositions (x^{az}) of the binary systems nonane + anisole and 1-pentanol + anisole at pressure (26.66, 53.33, 79.99, and 101.32) kPa are given in Table 5.

The azeotropic points have been determined from the function

$$\alpha_{12} = \frac{y_1/y_2}{x_1/x_2} \quad (5)$$

where y_i is the mole fraction of component i in the vapor phase, calculated by the Wilson equation and solving for $\alpha_{12} = 1$.

The isobaric VLE data for the ternary system are given in Table 6. Experimental $T-x$ values are presented together with calculated values of activity coefficients, vapor compositions, excess Gibbs energy, temperatures, and total pressures predicted by the Wilson equation. For example, the values of activity coefficients and the Gibbs energy G^E in ternary systems can expressed as

$$\gamma_i = \exp\left[1 - \ln\left(\sum_{j=1}^{3} x_j\Lambda_{ij}\right) - \sum_{k=1}^{3} \frac{x_k\Lambda_{ki}}{\sum_{j=1}^{3} x_j\Lambda_{kj}}\right] \quad (6)$$

where x_i is the mole fraction of component i.

Table 7. Azeotropic Boiling Temperature T_{az} and Compositions x_1^{az}, x_2^{az}, and x_3^{az} of the Ternary System 1-Pentanol (1) + Nonane (2) + Anisole (3) at a Pressure of 26.66 kPa

P/kPa	T_{az}/K	x_1^{az}	x_2^{az}	x_3^{az}
26.66	368.17	0.463	0.433	0.104

$$G^E = -RT\left[\sum_{i=1}^{3} x_i \ln \sum_{j=1}^{3} x_j\Lambda_{ij}\right] \quad (7)$$

Calculations have been made separately for (26.66, 53.33, 79.99, and 101.32) kPa pressures, using optimized values Λ_{12}, Λ_{21}, Λ_{23}, Λ_{32}, Λ_{13}, and Λ_{31}, by the simplex function minimization.[15] The optimized values differ from the values found in the calculations for binaries.

At the pressure 26.66 kPa, a strong interaction exists between components 1-pentanol, nonane, and anisole, which becomes weaker at higher pressures.

The ternary system exhibits at 26.66 kPa a minimum boiling azeotrope, for which composition was determined by the minimization of the function

$$(\alpha_{12} - 1) + (\alpha_{13} - 1) \Rightarrow \min \quad (8)$$

The parameters of the ternary azeotrope 1-pentanol (1) + nonane (2) + anisole (3) at 26.66 kPa are given in Table 7. At higher pressures investigated here, an azeotrope was not detected.

In Figure 3, the predicted boiling temperature isotherms for the ternary system 1-pentanol (1) + nonane (2) + anisole (3) at 26.66 kPa are presented on the Gibbs triangle.

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