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Liquid–Liquid Equilibria for 2-Phenylethan-1-ol + Alkane Systems

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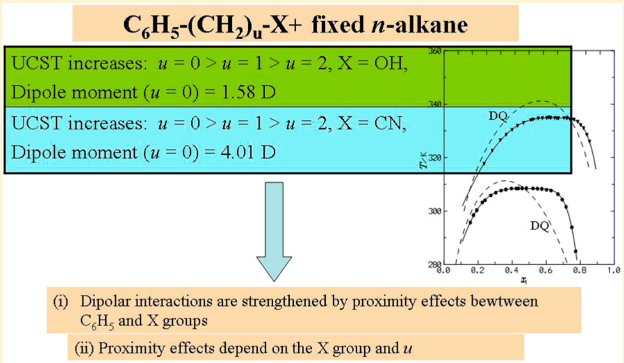
Supporting Information

ABSTRACT: The liquid–liquid equilibrium (LLE) curves for 2-phenylethan-1-ol (2-phenylethanol, 2PhEtOH) + octane, + decane, + dodecane, + tetradecane or + 2,2,4-trimethylpentane have been determined by a method of turbidimetry using a laser scattering technique. Experimental results reveal that the systems are characterized by an upper critical solution temperature (UCST), which increases linearly with the number of C atoms of the *n*-alkane. In addition, the LLE curves have a rather horizontal top and become skewed to higher mole fractions of the *n*-alkane, when its size increases. For a given *n*-alkane, UCST decreases as follows: phenol > phenylmethanol > 2-PhEtOH, indicating that dipolar interactions decrease in the same sequence. This has been ascribed to a weakening in the same order of the proximity effects between the phenyl and OH groups of the aromatic alkanols. DISQUAC interaction parameters for OH/aliphatic and OH/aromatic contacts in the investigated systems are reported. Phenol, or phenylmethanol or 2-PhEtOH, + *n*-alkane mixtures only differ by the first dispersive Gibbs energy interaction parameter for the (OH/aliphatic) contact.



1. INTRODUCTION

The investigation of liquid mixtures involving aromatic polar compounds is of great interest due to the proximity effects between the aromatic ring (C_6H_5 − group) and the polar X group of the aromatic compound. These effects are intramolecular effects and lead to interactions between the phenyl ring and the X group which are substantially different from those between the mentioned groups when they belong to different molecules.[1] In this framework, we have investigated mixtures including aromatic amines[2−9] (anilines, 2-amino-1-methylbenzene, 1-phenylmethanamine (benzylamine), 1*H*-pyrrole, quinoline or imizadoles), aromatic alkanals, ketones, or alkanoates,[1,10−12] and aromatic nitriles,[13] 2-phenoxyethanol,[14] or aromatic alkanols (phenol or phenylmethanol).[15,16] As continuation, we provide now liquid–liquid (LLE) measurements for binary systems formed by 2-phenylethan-1-ol (2-phenylethanol, 2PhEtOH) and octane, decane, dodecane, tetradecane, or 2,2,4-trimethylpentane.

2-PhEtOH is an aromatic alkanol characterized by its rose-like fragrance and widely used in the cosmetics, perfumery, and food industries.[17,18] In the pharmaceutical industry, it is also employed due to its antimicrobial properties. Interestingly, 2-PhEtOH is an intermediate in the microbial transformation of L-phenylalanine, an essential amino acid for humans. This makes possible a low cost production of 2-PhEtOH by enzymatic transformation or microbial fermentation through a natural process where difficult purification problems related to the chemical synthesis are avoided.[17,19]

2. EXPERIMENTAL SECTION

2.1. Materials. Information on source, purity, water contents, determined by the Karl Fischer method, and density (ρ) of the pure chemicals employed along this investigation is collected in Table 1. All the chemicals were used as received. Density values were obtained from a vibrating-tube densimeter and a sound analyzer, Anton Paar model DSA-5000. The repeatability of the ρ measurements is 5×10^{-3} kg·m^{-3}, while their relative standard uncertainty is 0.001. Inspection of Table 1 shows that there is a good agreement between our density results and those taken from the literature.

2.2. Apparatus and Procedure. Mixtures were prepared by mass in small Pyrex tubes of the following dimensions: 0.009 m i.d. and about 0.04 m length (free volume of the ampule ≈1.17×10^{-6} m^3). The tubes were immediately sealed by capping at 0.1 MPa and 298.15 K. Weights were measured using an analytical balance Sartorius NSU125p (weighing accuracy 10^{-8} kg). Mole fractions were calculated on the basis of the relative atomic mass Table of 2015 issued by the

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Table 1. Properties of Pure Compounds at 0.1 MPa and 298.15 K[a]

compound	CAS	source	initial mole fraction	ρ/kg·m^{-3a} exp.	ρ/kg·m^{-3a} lit.	water content[b]
2-phenylethanol	60-12-8	Sigma-Aldrich	≥99.9%[c]	1016.2	1016.1[45]	11×10^{-4}
octane	111-65-9	Sigma-Aldrich	≥99%.4[c]	698.71	698.62[46]	35×10^{-4}
decane	124-18-5	Fluka	≥99.8%[c]	726.35	726.35[46]	20×10^{-4}
dodecane	112-40-3	Fluka	≥99.7%[d]	745.51	745.32[47]	25×10^{-4}
tetradecane	629-59-4	Fluka	≥99.5%[c]	759.27	759.32[447]	25×10^{-4}
2,2,4-trimethylpentane	540-84-1	Fluka	≥99.9%[c]	687.32	687.81[46]	28×10^{-4}

[a] Standard uncertainties are $u(T)$ = 0.01 K; $u(P)$ = 0.5 kPa; the relative standard uncertainty for density is $u_r(\rho)$ = 0.001 and 0.02 for water content. [b] In mass fraction. [c] Provided by the supplier by gas chromatography. [d] By mass spectrometry.

Table 2. Experimental Liquid–Liquid Equilibrium Temperatures for 2-Phenylethanol (1) + Alkane(2) Mixtures[a] at 0.1 MPa

x_1	T/K	x_1	T/K
2-Phenylethanol (1) + Octane (2)			
0.1544	295.7	0.4835	308.5
0.1730	298.5	0.5223	308.5
0.1918	300.3	0.5485	308.4
0.2248	303.2	0.5742	308.3
0.2407	304.0	0.6019	307.9
0.2745	305.9	0.6281	307.7
0.3044	306.9	0.6487	306.9
0.3355	307.7	0.6684	306.3
0.3626	308.1	0.6943	304.3
0.3956	308.4	0.7165	301.6
0.4240	308.5	0.7502	293.9
0.4362	308.5	0.7730	285.0
0.4595	308.5		
2-Phenylethanol (1) + Decane (2)			
0.1822	303.0	0.5145	317.0
0.2007	305.1	0.54450	317.0
0.2318	308.1	0.5751	316.9
0.2471	309.6	0.5940	316.7
0.2708	311.3	0.6172	316.7
0.2942	312.8	0.6653	316.0
0.3365	314.7	0.6660	316.2
0.3617	315.3	0.6872	315.6
0.3807	315.7	0.7177	314.4
0.4197	316.6	0.7433	312.6
0.4466	316.6	0.7659	310.2
0.4692	316.8	0.7871	306.7
0.4991	317.0	0.8020	303.8
2-Phenylethanol (1) + Dodecane (2)			
0.1908	309.4	0.5996	326.0
0.2483	314.8	0.6247	326.0
0.2676	316.4	0.6405	325.8
0.2923	318.3	0.6733	325.7
0.3352	321.1	0.7062	325.4
0.3570	322.3	0.7251	325.1
0.3960	323.7	0.7486	324.2
0.4303	324.9	0.7728	322.7
0.4524	325.1	0.7970	320.7
0.4779	325.4	0.8277	317.5

x_1	T/K	x_1	T/K
2-Phenylethanol (1) + Dodecane (2)			
0.5052	325.7	0.8463	314.2
0.5271	325.8	0.8657	310.2
0.5573	325.9	0.8968	303.1
0.5840	325.9		
2-Phenylethanol (1) + Tetradecane (2)			
0.2155	317.8	0.6250	334.8
0.2833	322.7	0.6499	334.9
0.3312	326.6	0.6632	334.7
0.3652	328.7	0.6721	334.8
0.4002	330.5	0.7050	334.9
0.4317	331.9	0.7220	334.7
0.4672	333.1	0.7396	334.4
0.5104	334.0	0.7631	334.2
0.5225	334.3	0.7852	333.4
0.5527	334.7	0.8024	332.2
0.5771	334.9	0.8195	331.0
0.6028	334.8	0.8390	328.5
0.6128	335.0	0.8541	326.0
0.6223	335.0		
2-Phenylethanol (1) + 2,2,4-Trimethylpentane (2)			
0.1608	310.3	0.4532	322.4
0.1800	312.9	0.4805	322.5
0.2048	315.6	0.5021	322.4
0.2275	317.3	0.5298	322.2
0.2609	319.0	0.5457	322.3
0.2771	319.8	0.5793	322.1
0.3072	320.8	0.6009	321.6
0.3137	321.0	0.6317	320.7
0.3361	321.4	0.6464	320.1
0.3512	321.9	0.6742	317.7
0.3771	322.1	0.7534	306.7
0.4044	322.3	0.7742	302.0
0.4214	322.2		

[a] Standard uncertainties are $u(x_1)$ = 0.0030; $u(p)$ = 0.5 kPa; the combined expanded uncertainty (0.95 level of confidence) for temperature is $U_c(T)$ = 0.2 K in the flat region of the curves and 0.4 K outside this region.

Commission on Isotopic Abundances and Atomic Weights (IUPAC).[20]

The coexistence curves of liquid–liquid equilibrium were determined by a method of turbidimetry, that is, by means of the observation of the turbidity produced on cooling (1.2 K·h^{-1}) when a second phase takes place. The process is repeated at least three times. We have previously reported details on the experimental technique.[14] The equilibrium temperatures were measured using a Pt-1000 resistance. The thermometer was calibrated according to the ITS-90 scale of temperature and the triple point of the water and the fusion point of Ga were considered the fixed points. The precision of the equilibrium temperature measurements is ±0.001 K. The estimated standard uncertainties in the flat region of the coexistence curves, and outside of this region are is 0.1 and 0.2 K, respectively. The standard uncertainty of the equilibrium mole fraction is 0.0030. This value is determined taking into account that the more volatile component is partially evaporated to the mentioned free volume of the ampule.

3. EXPERIMENTAL RESULTS

Experimental results determined in this work, the directly measured liquid–liquid equilibrium temperatures, T, versus x_1, the mole fraction of 2-PhEtOH, for the systems with n-C_8, n-C_{10}, n-C_{12}, n-C_{14}, or 2,2,4,-trimethylpentane, are collected in Table 2 (Figure 1). As in many systems previously investigated,[1,3−5,9,11−16] the LLE curves of the present mixtures are characterized by some typical features: (i) they show a rather flat maximum (Figure 1); (ii) the curves become progressively skewed toward higher x_1 values when the chain length of the alkane is increased (Figure 1); (iii) the upper critical solution temperature, UCST increases with the number of C atoms of the n-alkane (Table 3).

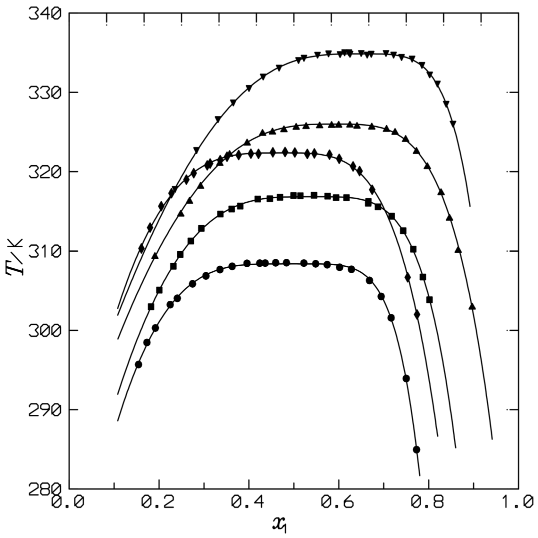

Figure 1. LLE for 2-phenylethanol(1) + octane(2) (●); + decane(2) (■); + dodecane(2) (▲); + tetradecane(2) (▼), or +2,2,4-trimethylpentane (◆) systems. Points, experimental results (this work); solid lines, calculations using the parameters listed in Table 3.

The experimental (x_1, T) data of each system were correlated by means of the equation[21,22]

$$T/K = T_c/K + k|y - y_c|^m \quad (1)$$

where

$$y = \frac{\alpha x_1}{1 + x_1(\alpha - 1)} \quad (2)$$

$$y_c = \frac{\alpha x_{1c}}{1 + x_{1c}(\alpha - 1)} \quad (3)$$

In these equations, m, k, α, T_c, and x_{1c} stand for the parameters which must be adjusted against the experimental data. The coordinates of the critical point are denoted by (x_{1c}, T_c). It is remarkable that when $\alpha = 1$, eq 1 is similar to[23−25]

$$\Delta\lambda = B\tau^{\beta} \quad (4)$$

In eq 4, $\Delta\lambda_1 = \lambda_1' - \lambda_2''$ is any order parameter, that is, any density variable in the conjugate phase. Particularly, in this research, $\lambda_1 = x_1$. In addition, τ (= $T_c - T)/T_c$) is the reduced temperature and β is the critical exponent related to$\Delta\lambda_1$. It is well-known that the critical exponent β depends on the theory applied to its determination.[23,26]

The m, k, α, T_c, and x_{1c} parameters were determined through an adjustment based on a Marquardt algorithm[27] with all the points weighted equally. Final values of m, k, α, T_c, and x_{1c} and of the standard deviations for LLE temperatures, $\sigma(T)$, are given in Table 3. The $\sigma(T)$ values are calculated from

$$(\sigma(T)/K) = \left[\sum (T_{exp}/K - T_{calc}/K)^2/(N - n)\right]^{1/2} \quad (5)$$

Here, N denotes the number of data points, and n (= 5) denotes the number of adjusted parameters. Results listed in Table 3 show that eq 1 fits well the experimental measurements.

The UCST for the 2,2,4-trimethylpentane system is available in the literature.[28] The value, 322.15 K, is in rather good agreement with our result (322.9 K, Table 3). A part of the observed difference may be due to the use of the method of equal volumes and solvent applied in the determination of the literature value of UCST, where, in addition, no information is provided about the rate of temperature change.

4. DISCUSSION

Below we are reporting values of excess molar enthalpies, H_m^E, at equimolar composition and 298.15 K. Moreover, we consider aromatic polar compounds of the type: $C_6H_5 - (CH_2)_u - X$ (X

Table 3. Coefficients in Equation 1 for the Fitting of the (x_1, T) Pairs Listed in Table 2 for 2-Phenylethanol (1) + Alkane(2) Mixtures; $\sigma(T)$ is the Standard Deviation Defined by Equation 5

N[a]	m	k	α	T_c/K	x_{1c}	$\sigma(T)$/K
			2-Phenylethanol(1) + Octane(2)			
24	4.471	− 5265	0.533	308.4 (311.3)[b]	0.499 (0.343)[b]	0.16
			2-phenylethanol(1) + Decane(2)			
26	3.761	− 1322	0.597	316.8 (317.3)[b]	0.543 (0.431)[b]	0.13
			2-Phenylethanol(1) + Dodecane(2)			
27	3.218	− 543	0.586	326.0 (330.4)[b]	0.593 (0.506)[b]	0.17
			2-Phenylethanol(1) + Tetradecane(2)			
27	3.583	− 952	0.419	334.8 (341.2)[b]	0.651 (0.573)[b]	0.11
			2-Phenylethanol(1) + 2,2,4-Trimethylpentane(2)			
25	3.571	− 1200	0.743	322.4	0.471	0.18

[a] Number of experimental data points. [b] DISQUAC value obtained using interchange coefficients listed in Table 4.

= OH, NH_2, CN, NO_2, CHO), or $C_6H_5 - (CH_2)_u - X - CH_3$ (X = CO, OCO) with different u values.

First, we remark the very different behavior of mixtures formed by 1-alkanol or aromatic alkanol and one n-alkane. Systems involving 1-alkanols are characterized by rather low H_m^E values. Thus, H_m^E (n-C_7)/J·mol^{-1} = 487 (heptan-1-ol);[29] 462 (octan-1-ol).[30] In addition, the H_m^E curves are skewed toward low alcohol concentrations.[29−31] These features have been explained in terms of the alcohol self-association, which is scarcely broken by alkanes. In contrast, mixtures containing aromatic alkanols show LLE curves, with moderately high UCST values (Figures 2-4). This clearly reveals that the dipolar interactions between alkanol molecules are strengthened by the presence of the C_6H_5− and −OH groups in the same molecule. Interestingly, the replacement of the n-alkane by an aromatic compound, say benzene, in mixtures with a given 1-alkanol leads to increased H_m^E values. For example; H_m^E (benzene)/J·mol^{-1} = 1109 (hexan-1-ol);[32] 1130 (octan-1-ol).[33] That is, aromatic compounds are more active molecules than n-alkanes when breaking the alcohol network. In summary, intermolecular effects between the −OH and aromatic groups increase H_m^E values compared to those of 1-alkanol + n-alkane systems, while intramolecular effects between the mentioned groups lead to solutions become more immiscible.

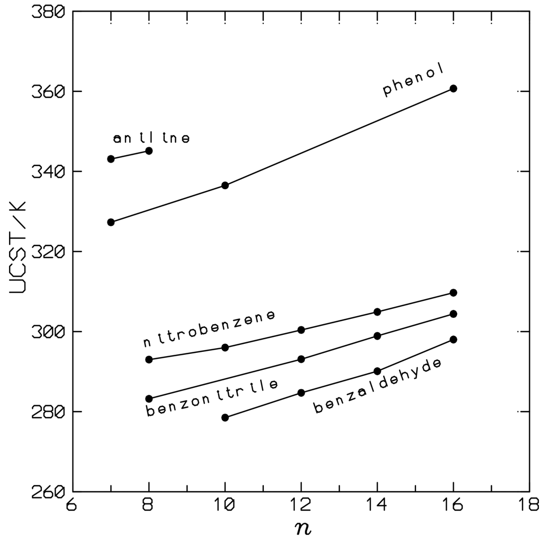

Figure 2. Upper critical solution temperatures, UCST for $C_6H_5 - X(1) + n$-alkane(2) systems (X = OH, NH_2, CN, NO_2, CHO), versus n, the number of C atoms in the alkane. Lines are only for the aid of the eye. For experimental data, see aniline,[34,48] phenol,[35,49,50] nitrobenzene,[51−55] benzonitrile,[36,56−58] and benzaldehyde.[11]

The strength of the intramolecular effects between the C_6H_5− and the X groups depends on the polar group considered. Figure 2 shows that UCST/K values of mixtures formed by an n-alkane and an aromatic polar component with u = 0 change in the order: 343.1 (aniline + heptane)[34] > 327.3 (phenol + heptane)[35] > 283.2 (benzonitrile + octane)[36] > 278.5 (benzaldehyde + decane).[11] In contrast, the corresponding μ/D values change in the sequence: 4.01 (benzonitrile) > 3 (benzaldehyde) > 1.58 (phenol) ≈ (1.57) aniline (Table S1, Supporting Information).[37] The observed variation of UCST with μ reveals that dipolar interactions are not merely related to the μ value of the polar compound, but they are also closely related to the proximity effects, which are stronger in solutions with phenol or aniline. In addition, self-association effects seem to be not very important as the UCST values of systems with the less self-associated aniline are higher than those of phenol mixtures (Figure 2). Nevertheless, the behavior described above may be different when the involved polar compound is characterized by $u \neq 0$, depending on the specific group. This is shown in Figures 3 and 4, where one can see that UCST values of solutions containing aromatic nitriles, rather polar compounds (Table Table S1, Supporting Information), are

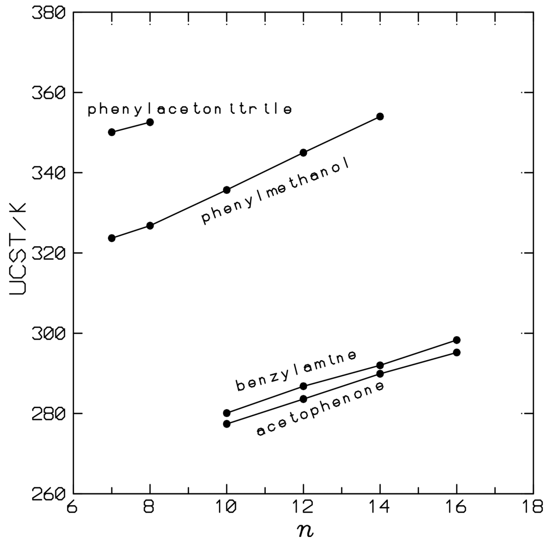

Figure 3. Upper critical solution temperatures, UCST for $C_6H_5 - CH_2 - X(1)$, or $C_6H_5 - CH_2 - X - CH_3 + n$-alkane(2) systems (X = OH, NH_2, CN, CO), versus n, the number of C atoms in the alkane. Lines are only for the aid of the eye. For experimental data, see phenylacetonitrile,[13] phenylmethanol,[16] benzylamine,[5] and acetophenone.[10]

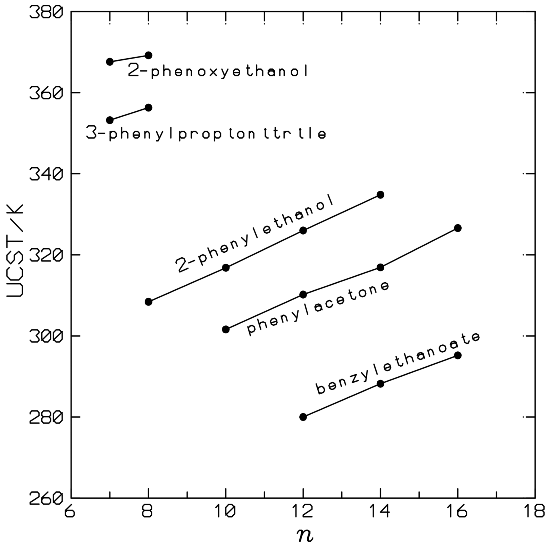

Figure 4. Upper critical solution temperatures, UCST for $C_6H_5 - (CH_2)_2 - X(1)$, or $C_6H_5 - (CH_2)_2 - X - CH_3(1)$, or 2-phenoxyethanol(1) + n-alkane(2) systems (X = OH, CN, CO, OCO), versus n, the number of C atoms in the alkane. Lines are only for the aid of the eye. For experimental data, see 3-phenylpropionitrile,[13] 2-phenylethanol (this work), 1-phenylpropan-2-one (phenylacetone),[1] benzylethanoate,[1,12] 2-phenoxyethanol.[14]

Table 4. Dispersive (DIS) and Quasichemical (QUAC) Interchange Coefficients, $C^{\mathrm{DIS}}_{\mathrm{st},l}$ and $C^{\mathrm{QUAC}}_{\mathrm{st},l}$, for (s,t) Contacts in (2-PhEtOH + *n*-Alkane) Mixtures (l = 1, Gibbs Energy; l = 2, Enthalpy; l = 3, Heat Capacity)

contact[a] (*s*,*t*)	$CH_3(CH_2)_nCH_3$	$C^{\mathrm{DIS}}_{st,1}$	$C^{\mathrm{DIS}}_{st,2}$	$C^{\mathrm{DIS}}_{st,3}$	$C^{\mathrm{QUAC}}_{st,1}$	$C^{\mathrm{QUAC}}_{st,2}$	$C^{\mathrm{QUAC}}_{st,3}$
(b,h)		4.80	− 2.65		5.70	13	
(a,h)	$n \leq 7$	3.55	0.50	− 5	11.25	16	12
(a,h)	$n = 8$	3.36	0.50	− 5	11.25	16	12
(a,h)	$n > 8$	3.36	0.50	5	11.25	16	30

[a] Type a, aliphatic in alkane, or 2-PhEtOH; type b, C_6H_5 in 2-PhEtOH; type h, OH, in 2-PhEtOH

higher than those of systems with aromatic alkanols or alkanones, benzylamine, or benzylethanoate. Therefore, the variation of UCTS with *u* for mixtures with a fixed alkane also depends on the group. Thus, UCST/K changes in the order: 327.3 (phenol (u = 0) + heptane)[35] > 323.7 (phenylmethanol (u = 1) + heptane)[16] > 308.4 (2-phenylethanol (u = 2) + octane) (this work), while UCST(octane)/K = 356.3 (3-phenylpropionitrile (u = 2))[13] > 352.6 (phenylacetonitrile (u = 1))[13] > 283.2 (benzonitrile (u = 0)).[36]

On the other hand, the replacement of octane by 2,2,4-trimethylpentane in systems with 2-PhEtOH leads to increased UCST values. This trend is also held for mixtures involving other aromatic polar compounds (phenol, nitriles, alkanones, or aniline).[13] Different results can be obtained depending on the nature of the solute and of the branching of the alkane, as we have shown from a detailed investigation on tertiary amide + alkane mixtures.[38]

It is pertinent to compare UCST values for mixtures with 2-PhEtOH or 2-phenoxyethanol (Figure 4). The latter have higher critical temperatures, which can be ascribed to such systems are also characterized by proximity effects between the O and OH groups.[39] Mixtures involving linear alkoxyethanols also show higher UCST values than the corresponding mixtures with homomorphic 1-alkanols. For example, for the 2-methoxyethanol + heptane system, UCST = 319.7 K,[40] while $H^{\mathrm{E}}_{\mathrm{m}}/\mathrm{J\cdot mol^{-1}}$ of the mixture penta-1-ol (isomeric alkanol of 2-methoxyethanol) + heptane is 575.[41]

Finally, we have applied the DISQUAC group contribution model[42,43] to represent the LLE curves of the 2-PhEtOH + *n*-alkane systems (Figure 1, Supporting Information). The main features of the model can be found elsewhere.[42,43] Here, we merely remark on the following: (i) The geometrical parameters of the groups referred in the work, C_6H_5, aliphatic, and OH, are available in the literature.[15] (ii) The temperature dependence of the interaction parameters is described by means of DIS (dispersive) and QUAC (quasichemical) interchange coefficients,[42,43] $C^{\mathrm{DIS}}_{st,l}$; $C^{\mathrm{QUAC}}_{st,l}$ where $s \neq t$ are two contact surfaces present in the mixture and l = 1 (Gibbs energy); l = 2 (enthalpy); l = 3 (heat capacity). (iii) 2-PhEtOH + *n*-alkane mixtures are built by the following surfaces: type a, aliphatic (CH_3, CH_2, in *n*-alkanes, or 2-PhEtOH); type b, aromatic (C_6H_5 in 2-PhEtOH), and type h, hydroxyl (OH in 2-PhEtOH). These surfaces generate three contacts: (a,b); (a,h), and (b,h). The (a,b) contact is characterized by purely dispersive interaction parameters, previously determined from the study of alkyl-benzene + alkane mixtures.[44] In contrast, interactions parameters for the (a,h) and (b,h) contacts are represented by both DIS and QUAC interchange coefficients. (iv) In our work on phenylmethanol + *n*-alkane systems,[16] we showed that the corresponding coordinates of the critical points can be fairly well described using the values of $C^{\mathrm{DIS}}_{\mathrm{bh},l}$, $C^{\mathrm{DIS}}_{\mathrm{sh},l}$ (s = a, b; l = 2, 3), and $C^{\mathrm{QUAC}}_{\mathrm{sh},l}$ (s = a, b and l = 1, 2, 3) of the phenol mixtures, and merely fitting the coefficient $C^{\mathrm{DIS}}_{\mathrm{ah},1}$. Here, we have applied the same approach. The final interaction parameters are listed in Table 4. DISQUAC results obtained for (x_{1c}, T_c) are listed in Table 3. The coordinates of the critical points are described in the correct range of composition and temperature, although our theoretical LLE curves are more rounded than the experimental ones (Figure S1, Supporting Information). This can be explained taking into account that DISQUAC calculations are conducted assuming erroneously that the excess functions are analytical in the vicinity of the critical points, although really, at the mentioned condition, thermodynamic properties follow scaling laws with universal critical exponents and universal scaling functions.[23] More details on this regard can be found elsewhere.[16] We conclude remarking that our DISQUAC results suggest that systems including an aromatic alkanol of the type $C_6H_5 - (CH_2)_u - OH$ (u = 0, 1, 2) can be characterized by the same QUAC interaction parameters for the OH/aliphatic and OH/aromatic contacts, and form an homologous series. The mixtures aniline[2] or 2-methylaniline[5] + alkane behave similarly.

5. CONCLUSIONS

Liquid−liquid equilibrium temperatures versus composition have been experimentally determined for 2-PhEtOH + octane, + decane, + dodecane, + tetradecane, or + 2,2,4-trimethylpentane systems. All the curves show a UCST, which increases linearly with the alkane size. Proximity effects become weaker in the sequence: phenol > phenylmethanol > 2- PhEtOH. DISQUAC interaction parameters are reported for 2-PhEtOH + *n*-alkane systems. Mixtures with phenol, phenylmethanol, or 2-phenylethanol are characterized by the same $C^{\mathrm{QUAC}}_{\mathrm{sh},l}$ (s = a, b; l = 1, 2, 3) and $C^{\mathrm{DIS}}_{\mathrm{sh},l}$ (s = a, b; l = 2, 3) coefficients, while differ only by the $C^{\mathrm{DIS}}_{\mathrm{ah},1}$ coefficients.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jced.7b00869.

Table S1 lists dipole moments of aromatic polar compounds considered along the work; Figure S1 shows a comparison between experimental results and DISQUAC calculations (PDF)

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Notes

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