

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

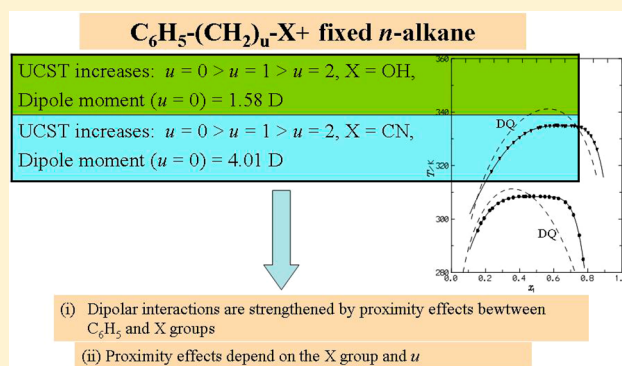
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## Supporting Information

**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<sub>6</sub>H<sub>5</sub> – 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.<sup>1</sup> In this framework, we have investigated mixtures including aromatic amines<sup>2–9</sup> (anilines, 2-amino-1-methylbenzene, 1-phenylmethanamine (benzylamine), 1H-pyrrole, quinoline or imizadoles), aromatic alkanals, ketones, or alkanooates,<sup>1,10–12</sup> and aromatic nitriles,<sup>13</sup> 2-phenoxyethanol,<sup>14</sup> or aromatic alkanols (phenol or phenylmethanol).<sup>15,16</sup> 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.<sup>17,18</sup> 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.<sup>17,19</sup>

## 2. EXPERIMENTAL SECTION

**2.1. Materials.** Information on source, purity, water contents, determined by the Karl Fischer method, and density ( $\rho$ ) 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  $\rho$  measurements is  $5 \times 10^{-3} \text{ kg}\cdot\text{m}^{-3}$ , 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  $\approx 1.17 \times 10^{-6} \text{ m}^3$ ). The tubes were immediately sealed by capping at 0.1 MPa and 298.15 K. Weights were measured using an analytical balance Sartorius NSU12Sp (weighing accuracy  $10^{-8} \text{ kg}$ ). 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<sup>a</sup>

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

<sup>a</sup>Standard uncertainties are  $u(T) = 0.01 \text{ K}$ ;  $u(P) = 0.5 \text{ kPa}$ ; the relative standard uncertainty for density is  $u_r(\rho) = 0.001$  and 0.02 for water content.

<sup>b</sup>In mass fraction. <sup>c</sup>Provided by the supplier by gas chromatography. <sup>d</sup>By mass spectrometry.

Table 2. Experimental Liquid–Liquid Equilibrium Temperatures for 2-Phenylethanol (1) + Alkane(2) Mixtures<sup>a</sup> at 0.1 MPa

$x_1$	T/K	$x_1$	T/K	$x_1$	T/K	$x_1$	T/K
2-Phenylethanol (1) + Octane (2)				2-Phenylethanol (1) + Dodecane (2)			
0.1544	295.7	0.4835	308.5	0.5052	325.7	0.8463	314.2
0.1730	298.5	0.5223	308.5	0.5271	325.8	0.8657	310.2
0.1918	300.3	0.5485	308.4	0.5573	325.9	0.8968	303.1
0.2248	303.2	0.5742	308.3	0.5840	325.9		
0.2407	304.0	0.6019	307.9	2-Phenylethanol (1) + Tetradecane (2)			
0.2745	305.9	0.6281	307.7	0.2155	317.8	0.6250	334.8
0.3044	306.9	0.6487	306.9	0.2833	322.7	0.6499	334.9
0.3355	307.7	0.6684	306.3	0.3312	326.6	0.6632	334.7
0.3626	308.1	0.6943	304.3	0.3652	328.7	0.6721	334.8
0.3956	308.4	0.7165	301.6	0.4002	330.5	0.7050	334.9
0.4240	308.5	0.7502	293.9	0.4317	331.9	0.7220	334.7
0.4362	308.5	0.7730	285.0	0.4672	333.1	0.7396	334.4
0.4595	308.5			0.5104	334.0	0.7631	334.2
2-Phenylethanol (1) + Decane (2)				0.5225	334.3	0.7852	333.4
0.1822	303.0	0.5145	317.0	0.5527	334.7	0.8024	332.2
0.2007	305.1	0.54450	317.0	0.5771	334.9	0.8195	331.0
0.2318	308.1	0.5751	316.9	0.6028	334.8	0.8390	328.5
0.2471	309.6	0.5940	316.7	0.6128	335.0	0.8541	326.0
0.2708	311.3	0.6172	316.7	0.6223	335.0		
0.2942	312.8	0.6653	316.0	2-Phenylethanol (1) + 2,2,4-Trimethylpentane (2)			
0.3365	314.7	0.6660	316.2	0.1608	310.3	0.4532	322.4
0.3617	315.3	0.6872	315.6	0.1800	312.9	0.4805	322.5
0.3807	315.7	0.7177	314.4	0.2048	315.6	0.5021	322.4
0.4197	316.6	0.7433	312.6	0.2275	317.3	0.5298	322.2
0.4466	316.6	0.7659	310.2	0.2609	319.0	0.5457	322.3
0.4692	316.8	0.7871	306.7	0.2771	319.8	0.5793	322.1
0.4991	317.0	0.8020	303.8	0.3072	320.8	0.6009	321.6
2-Phenylethanol (1) + Dodecane (2)				0.3137	321.0	0.6317	320.7
0.1908	309.4	0.5996	326.0	0.3361	321.4	0.6464	320.1
0.2483	314.8	0.6247	326.0	0.3512	321.9	0.6742	317.7
0.2676	316.4	0.6405	325.8	0.3771	322.1	0.7534	306.7
0.2923	318.3	0.6733	325.7	0.4044	322.3	0.7742	302.0
0.3352	321.1	0.7062	325.4	0.4214	322.2		
0.3570	322.3	0.7251	325.1	<sup>a</sup> Standard uncertainties are $u(x_1) = 0.0030$ ; $u(p) = 0.5 \text{ kPa}$ ; the combined expanded uncertainty (0.95 level of confidence) for temperature is $U_c(T) = 0.2 \text{ K}$ in the flat region of the curves and 0.4 K outside this region.			
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				

70 Commission on Isotopic Abundances and Atomic Weights  
71 (IUPAC).<sup>20</sup>

72 The coexistence curves of liquid–liquid equilibrium were  
73 determined by a method of turbidimetry, that is, by means of  
74 the observation of the turbidity produced on cooling (1.2 K·  
75 h<sup>-1</sup>) when a second phase takes place. The process is repeated  
76 at least three times. We have previously reported details on the

experimental technique.<sup>14</sup> The equilibrium temperatures were  
77 measured using a Pt-1000 resistance. The thermometer was  
78 calibrated according to the ITS-90 scale of temperature and the  
79 triple point of the water and the fusion point of Ga were  
80 considered the fixed points. The precision of the equilibrium  
81 temperature measurements is  $\pm 0.001 \text{ K}$ . The estimated  
82 standard uncertainties in the flat region of the coexistence  
83

84 curves, and outside of this region are 0.1 and 0.2 K,  
85 respectively. The standard uncertainty of the equilibrium mole  
86 fraction is 0.0030. This value is determined taking into account  
87 that the more volatile component is partially evaporated to the  
88 mentioned free volume of the ampule.

### 3. EXPERIMENTAL RESULTS

89 Experimental results determined in this work, the directly  
90 measured liquid–liquid equilibrium temperatures,  $T$ , versus  $x_1$ ,  
91 the mole fraction of 2-PhEtOH, for the systems with  $n$ -C<sub>8</sub>,  $n$ -  
92 C<sub>10</sub>,  $n$ -C<sub>12</sub>,  $n$ -C<sub>14</sub>, or 2,2,4-trimethylpentane, are collected in  
93 Table 2 (Figure 1). As in many systems previously

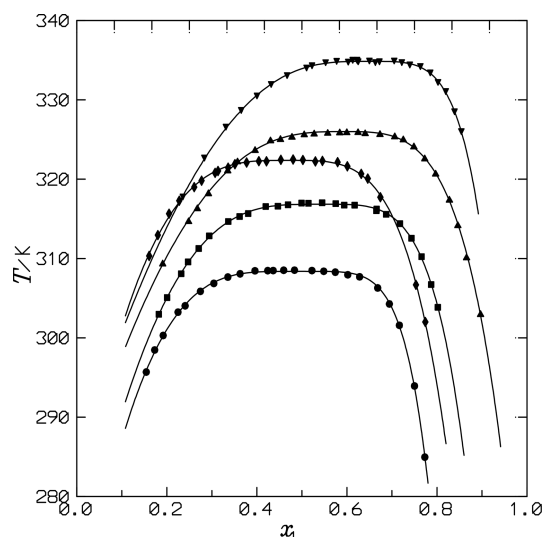


Figure 1. LLE for 2-phenylethanol(1) + octane(2) (●); + decane(2) (■); + dodecane(2) (▲); + tetradecane(2) (▼), or +2,2,4-trimethylpentane (◆) systems. Points, experimental results (this work); solid lines, calculations using the parameters listed in Table 3.

94 investigated,<sup>1,3–5,9,11–16</sup> the LLE curves of the present mixtures  
95 are characterized by some typical features: (i) they show a  
96 rather flat maximum (Figure 1); (ii) the curves become  
97 progressively skewed toward higher  $x_1$  values when the chain  
98 length of the alkane is increased (Figure 1); (iii) the upper  
99 critical solution temperature, UCST increases with the number  
100 of C atoms of the  $n$ -alkane (Table 3).

101 The experimental ( $x_1, T$ ) data of each system were correlated  
102 by means of the equation<sup>21,22</sup>

$$T/K = T_c/K + k|y - y_c|^m \quad (1) \quad 103$$

where 104

$$y = \frac{\alpha x_1}{1 + x_1(\alpha - 1)} \quad (2) \quad 105$$

$$y_c = \frac{\alpha x_{1c}}{1 + x_{1c}(\alpha - 1)} \quad (3) \quad 106$$

In these equations,  $m$ ,  $k$ ,  $\alpha$ ,  $T_c$ , and  $x_{1c}$  stand for the parameters  
107 which must be adjusted against the experimental data. The  
108 coordinates of the critical point are denoted by ( $x_{1c}, T_c$ ). It is  
109 remarkable that when  $\alpha = 1$ , eq 1 is similar to<sup>23–25</sup>  
110

$$\Delta\lambda = B\tau^\beta \quad (4) \quad 111$$

In eq 4,  $\Delta\lambda_1 = \lambda_1' - \lambda_2''$  is any order parameter, that is, any  
112 density variable in the conjugate phase. Particularly, in this  
113 research,  $\lambda_1 = x_1$ . In addition,  $\tau = (T_c - T)/T_c$  is the reduced  
114 temperature and  $\beta$  is the critical exponent related to  $\Delta\lambda_1$ . It  
115 is well-known that the critical exponent  $\beta$  depends on the theory  
116 applied to its determination.<sup>23,26</sup>  
117

The  $m$ ,  $k$ ,  $\alpha$ ,  $T_c$ , and  $x_{1c}$  parameters were determined through  
118 an adjustment based on a Marquardt algorithm<sup>27</sup> with all the  
119 points weighted equally. Final values of  $m$ ,  $k$ ,  $\alpha$ ,  $T_c$ , and  $x_{1c}$   
120 and of the standard deviations for LLE temperatures,  $\sigma(T)$ , are  
121 given in Table 3. The  $\sigma(T)$  values are calculated from  
122

$$(\sigma(T)/K) = \left[ \sum (T_{\text{exp}}/K - T_{\text{calc}}/K)^2 / (N - n) \right]^{1/2} \quad (5) \quad 123$$

Here,  $N$  denotes the number of data points, and  $n$  ( $= 5$ )  
124 denotes the number of adjusted parameters. Results listed in  
125 Table 3 show that eq 1 fits well the experimental measure-  
126 ments.  
127

The UCST for the 2,2,4-trimethylpentane system is available  
128 in the literature.<sup>28</sup> The value, 322.15 K, is in rather good  
129 agreement with our result (322.9 K, Table 3). A part of the  
130 observed difference may be due to the use of the method of  
131 equal volumes and solvent applied in the determination of the  
132 literature value of UCST, where, in addition, no information is  
133 provided about the rate of temperature change.  
134

### 4. DISCUSSION

Below we are reporting values of excess molar enthalpies,  $H_m^E$ ,  
135 at equimolar composition and 298.15 K. Moreover, we consider  
136 aromatic polar compounds of the type: C<sub>6</sub>H<sub>5</sub> – (CH<sub>2</sub>)<sub>*n*</sub> – X (X  
137

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

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

<sup>a</sup>Number of experimental data points. <sup>b</sup>DISQUAC value obtained using interchange coefficients listed in Table 4.

138 = OH, NH<sub>2</sub>, CN, NO<sub>2</sub>, CHO), or C<sub>6</sub>H<sub>5</sub> - (CH<sub>2</sub>)<sub>u</sub> - X - CH<sub>3</sub>,  
 139 (X = CO, OCO) with different *u* values.

140 First, we remark the very different behavior of mixtures  
 141 formed by 1-alkanol or aromatic alkanol and one *n*-alkane.  
 142 Systems involving 1-alkanols are characterized by rather low  $H_m^E$   
 143 values. Thus,  $H_m^E$  (*n*-C<sub>7</sub>)/J·mol<sup>-1</sup> = 487 (heptan-1-ol);<sup>29</sup> 462  
 144 (octan-1-ol).<sup>30</sup> In addition, the  $H_m^E$  curves are skewed toward  
 145 low alcohol concentrations.<sup>29–31</sup> These features have been  
 146 explained in terms of the alcohol self-association, which is  
 147 scarcely broken by alkanes. In contrast, mixtures containing  
 148 aromatic alkanols show LLE curves, with moderately high  
 149 UCST values (Figures 2–4). This clearly reveals that the dipolar

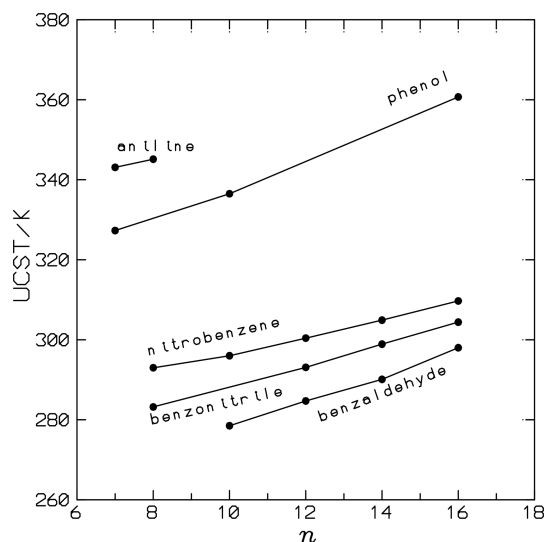


Figure 2. Upper critical solution temperatures, UCST for C<sub>6</sub>H<sub>5</sub> - X(1) + *n*-alkane(2) systems (X = OH, NH<sub>2</sub>, CN, NO<sub>2</sub>, CHO), versus *n*, the number of C atoms in the alkane. Lines are only for the aid of the eye. For experimental data, see aniline,<sup>34,48</sup> phenol,<sup>35,49,50</sup> nitrobenzene,<sup>51–55</sup> benzonitrile,<sup>36,56–58</sup> and benzaldehyde.<sup>11</sup>

150 interactions between alkanol molecules are strengthened by the  
 151 presence of the C<sub>6</sub>H<sub>5</sub>- and -OH groups in the same molecule.  
 152 Interestingly, the replacement of the *n*-alkane by an aromatic  
 153 compound, say benzene, in mixtures with a given 1-alkanol  
 154 leads to increased  $H_m^E$  values. For example;  $H_m^E$  (benzene)/J·  
 155 mol<sup>-1</sup> = 1109 (hexan-1-ol);<sup>32</sup> 1130 (octan-1-ol).<sup>33</sup> That is,  
 156 aromatic compounds are more active molecules than *n*-alkanes  
 157 when breaking the alcohol network. In summary, intermolec-  
 158 ular effects between the -OH and aromatic groups increase  $H_m^E$   
 159 values compared to those of 1-alkanol + *n*-alkane systems, while  
 160 intramolecular effects between the mentioned groups lead to  
 161 solutions become more immiscible.

162 The strength of the intramolecular effects between the  
 163 C<sub>6</sub>H<sub>5</sub>- and the X groups depends on the polar group  
 164 considered. Figure 2 shows that UCST/K values of mixtures  
 165 formed by an *n*-alkane and an aromatic polar component with *u*  
 166 = 0 change in the order: 343.1 (aniline + heptane)<sup>34</sup> > 327.3  
 167 (phenol + heptane)<sup>35</sup> > 283.2 (benzonitrile + octane)<sup>36</sup> > 278.5  
 168 (benzaldehyde + decane).<sup>11</sup> In contrast, the corresponding  $\mu/D$   
 169 values change in the sequence: 4.01 (benzonitrile) > 3  
 170 (benzaldehyde) > 1.58 (phenol)  $\approx$  (1.57) aniline (Table S1,  
 171 Supporting Information).<sup>37</sup> The observed variation of UCST  
 172 with  $\mu$  reveals that dipolar interactions are not merely related to  
 173 the  $\mu$  value of the polar compound, but they are also closely  
 174 related to the proximity effects, which are stronger in solutions

with phenol or aniline. In addition, self-association effects seem  
 175 to be not very important as the UCST values of systems with  
 176 the less self-associated aniline are higher than those of phenol  
 177 mixtures (Figure 2). Nevertheless, the behavior described above  
 178 may be different when the involved polar compound is  
 179 characterized by *u*  $\neq$  0, depending on the specific group.  
 180 This is shown in Figures 3 and 4, where one can see that UCST  
 181 184

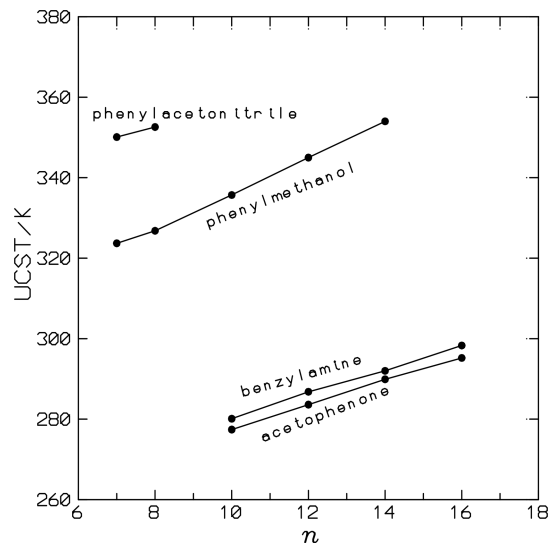


Figure 3. Upper critical solution temperatures, UCST for C<sub>6</sub>H<sub>5</sub> - CH<sub>2</sub> - X(1), or C<sub>6</sub>H<sub>5</sub> - CH<sub>2</sub> - X - CH<sub>3</sub> + *n*-alkane(2) systems (X = OH, NH<sub>2</sub>, CN, CO), versus *n*, the number of C atoms in the alkane. Lines are only for the aid of the eye. For experimental data, see phenylacetone nitrile,<sup>13</sup> phenylmethanol,<sup>16</sup> benzylamine,<sup>5</sup> and acetophenone.<sup>10</sup>

values of solutions containing aromatic nitriles, rather polar  
 182 compounds (Table Table S1, Supporting Information), are 183

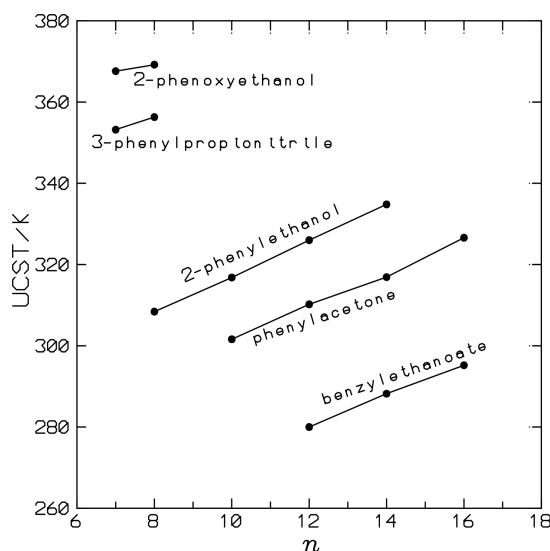


Figure 4. Upper critical solution temperatures, UCST for C<sub>6</sub>H<sub>5</sub> - (CH<sub>2</sub>)<sub>2</sub> - X(1), or C<sub>6</sub>H<sub>5</sub> - (CH<sub>2</sub>)<sub>2</sub> - X - CH<sub>3</sub>(1), or 2-phenoxyethanol(1) + *n*-alkane(2) systems (X = OH, CN, CO, OCO), versus *n*, the number of C atoms in the alkane. Lines are only for the aid of the eye. For experimental data, see 3-phenylpropan nitrile,<sup>13</sup> 2-phenylethanol (this work), 1-phenylpropan-2-one (phenylacetone),<sup>1</sup> benzylethanoate,<sup>1,12</sup> 2-phenoxyethanol.<sup>14</sup>

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

contact <sup>a</sup> (s,t)	CH <sub>3</sub> (CH <sub>2</sub> ) <sub><i>n</i></sub> CH <sub>3</sub>	$C_{st,1}^{\text{DIS}}$	$C_{st,2}^{\text{DIS}}$	$C_{st,3}^{\text{DIS}}$	$C_{st,1}^{\text{QUAC}}$	$C_{st,2}^{\text{QUAC}}$	$C_{st,3}^{\text{QUAC}}$
(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

<sup>a</sup>Type a, aliphatic in alkane, or 2-PhEtOH; type b, C<sub>6</sub>H<sub>5</sub> in 2-PhEtOH; type h, OH, in 2-PhEtOH

184 higher than those of systems with aromatic alkanols or  
185 alkanones, benzylamine, or benzylethanoate. Therefore, the  
186 variation of UCSTs with *u* for mixtures with a fixed alkane also  
187 depends on the group. Thus, UCST/K changes in the order:  
188 327.3 (phenol (*u* = 0) + heptane)<sup>35</sup> > 323.7 (phenylmethanol  
189 (*u* = 1) + heptane)<sup>16</sup> > 308.4 (2-phenylethanol (*u* = 2) +  
190 octane) (this work), while UCST(octane)/K = 356.3 (3-  
191 phenylpropionitrile (*u* = 2))<sup>13</sup> > 352.6 (phenylacetonitrile (*u* =  
192 1))<sup>13</sup> > 283.2 (benzonitrile (*u* = 0)).<sup>36</sup>

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

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

211 Finally, we have applied the DISQUAC group contribution  
212 model<sup>42,43</sup> to represent the LLE curves of the 2-PhEtOH + *n*-  
213 alkane systems (Figure 1, Supporting Information). The main  
214 features of the model can be found elsewhere.<sup>42,43</sup> Here, we  
215 merely remark on the following: (i) The geometrical  
216 parameters of the groups referred in the work, C<sub>6</sub>H<sub>5</sub>, aliphatic,  
217 and OH, are available in the literature.<sup>15</sup> (ii) The temperature  
218 dependence of the interaction parameters is described by  
219 means of DIS (dispersive) and QUAC (quasichemical)  
220 interchange coefficients,<sup>42,43</sup>  $C_{st,l}^{\text{DIS}}$ ;  $C_{st,l}^{\text{QUAC}}$  where  $s \neq t$  are two  
221 contact surfaces present in the mixture and  $l = 1$  (Gibbs  
222 energy);  $l = 2$  (enthalpy);  $l = 3$  (heat capacity). (iii) 2-PhEtOH  
223 + *n*-alkane mixtures are built by the following surfaces: type a,  
224 aliphatic (CH<sub>3</sub>, CH<sub>2</sub>, in *n*-alkanes, or 2-PhEtOH); type b,  
225 aromatic (C<sub>6</sub>H<sub>5</sub> in 2-PhEtOH), and type h, hydroxyl (OH in 2-  
226 PhEtOH). These surfaces generate three contacts: (a,b); (a,h),  
227 and (b,h). The (a,b) contact is characterized by purely  
228 dispersive interaction parameters, previously determined from  
229 the study of alkyl-benzene + alkane mixtures.<sup>44</sup> In contrast,  
230 interactions parameters for the (a,h) and (b,h) contacts are  
231 represented by both DIS and QUAC interchange coefficients.  
232 (iv) In our work on phenylmethanol + *n*-alkane systems,<sup>16</sup> we  
233 showed that the corresponding coordinates of the critical points  
234 can be fairly well described using the values of  $C_{bh,l}^{\text{DIS}}$ ,  $C_{sh,l}^{\text{DIS}}$  ( $s = a$ ,  
235 b;  $l = 2, 3$ ), and  $C_{sh,l}^{\text{QUAC}}$  ( $s = a, b$  and  $l = 1, 2, 3$ ) of the phenol  
236 mixtures, and merely fitting the coefficient  $C_{ah,1}^{\text{DIS}}$ . Here, we have

237 applied the same approach. The final interaction parameters are  
238 listed in Table 4. DISQUAC results obtained for ( $x_{1c}$ ,  $T_c$ ) are  
239 listed in Table 3. The coordinates of the critical points are  
240 described in the correct range of composition and temperature,  
241 although our theoretical LLE curves are more rounded than the  
242 experimental ones (Figure S1, Supporting Information). This  
243 can be explained taking into account that DISQUAC  
244 calculations are conducted assuming erroneously that the  
245 excess functions are analytical in the vicinity of the critical  
246 points, although really, at the mentioned condition, thermody-  
247 namic properties follow scaling laws with universal critical  
248 exponents and universal scaling functions.<sup>23</sup> More details on  
249 this regard can be found elsewhere.<sup>16</sup> We conclude remarking  
250 that our DISQUAC results suggest that systems including an  
251 aromatic alkanol of the type C<sub>6</sub>H<sub>5</sub> − (CH<sub>2</sub>)<sub>*u*</sub> − OH (*u* = 0, 1,  
252 2) can be characterized by the same QUAC interaction  
253 parameters for the OH/aliphatic and OH/aromatic contacts,  
254 and form an homologous series. The mixtures aniline<sup>2</sup> or 2-  
255 methylaniline<sup>5</sup> + alkane behave similarly.

## 5. CONCLUSIONS

256 Liquid–liquid equilibrium temperatures versus composition  
257 have been experimentally determined for 2-PhEtOH + octane,  
258 + decane, + dodecane, + tetradecane, or + 2,2,4-trimethylpen-  
259 tane systems. All the curves show a UCST, which increases  
260 linearly with the alkane size. Proximity effects become weaker  
261 in the sequence: phenol > phenylmethanol > 2-PhEtOH.  
262 DISQUAC interaction parameters are reported for 2-PhEtOH  
263 + *n*-alkane systems. Mixtures with phenol, phenylmethanol, or  
264 2-phenylethanol are characterized by the same  $C_{sh,l}^{\text{QUAC}}$  ( $s = a, b$ ;  $l = 2, 3$ )  
265 and  $C_{sh,l}^{\text{DIS}}$  ( $s = a, b$ ;  $l = 2, 3$ ) coefficients, while differ  
266 only by the  $C_{ah,1}^{\text{DIS}}$  coefficients.

## ■ ASSOCIATED CONTENT

### 📄 Supporting Information

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

269 Table S1 lists dipole moments of aromatic polar  
270 compounds considered along the work; Figure S1  
271 shows a comparison between experimental results and  
272 DISQUAC calculations (PDF)  
273  
274

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