

**Supporting Information**

**Thermodynamic Functions for Solubility of  
1-Hydroxybenzotriazole in Sixteen Solvents at temperatures  
from (278.15 to 313.15) K and Mixing Property of mixtures**

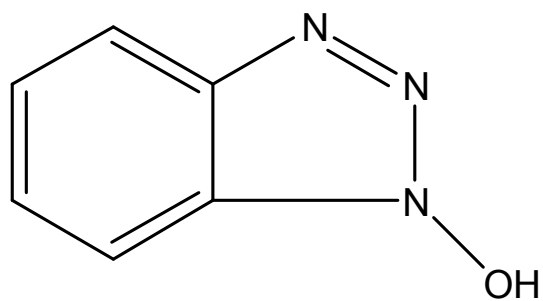
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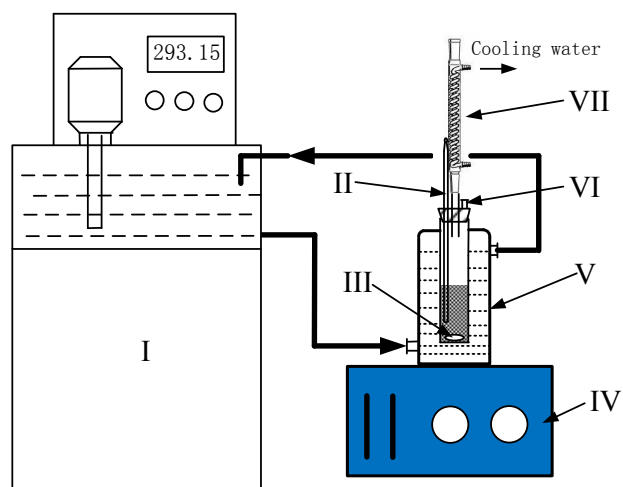
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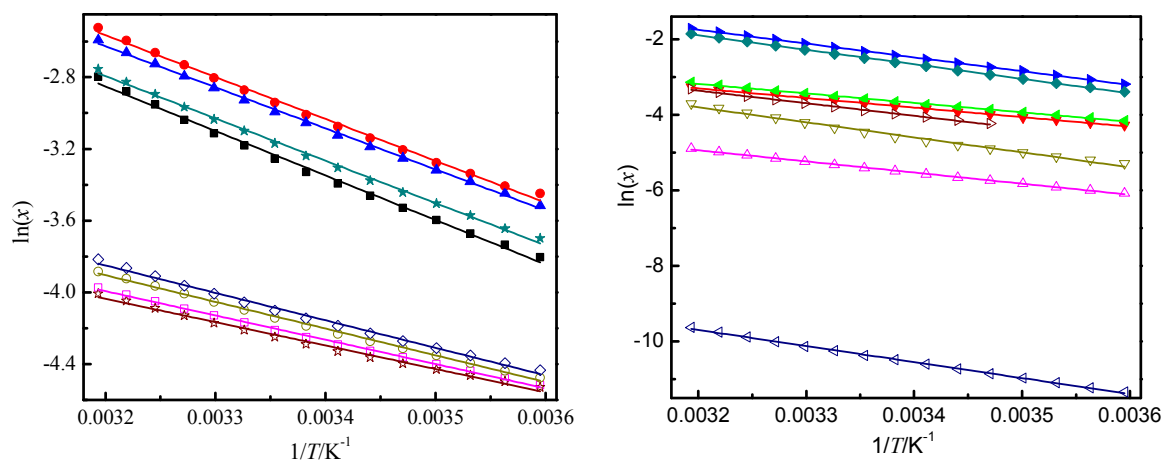
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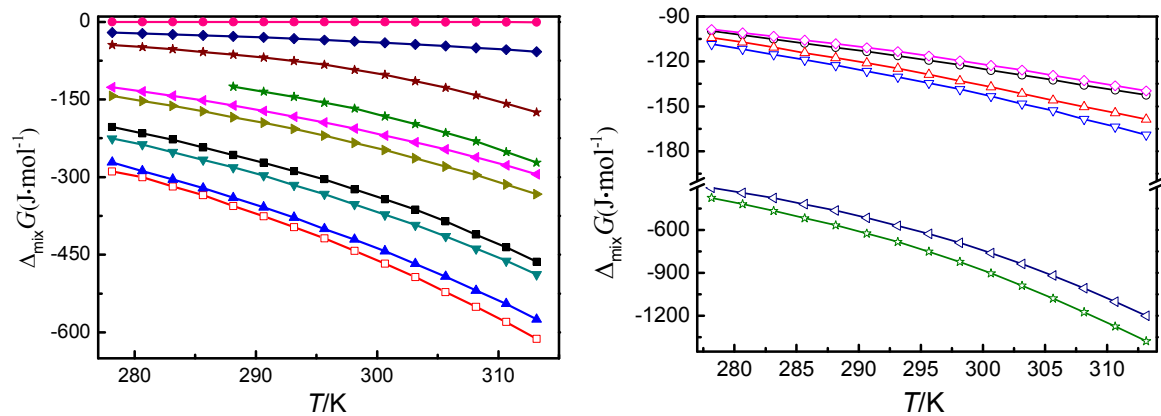
**Figure S1.** Chemical structure of 1-hydroxybenzotriazole.



**Figure S2.** Schematic diagram of experimental apparatus: I, smart thermostatic water bath; II, mercury-in-glass thermometer; III, magnetic stirrer; IV, stirrer controller; V, jacketed glass vessel; VI, sampling port; VII, condenser.



**Figure S3.** The van't Hoff plots of  $\ln(x)$  versus  $1/T$  in different solvents: ●, ethanol; ▲, *n*-propanol; ★, isopropanol; ■, methanol; ◇, *n*-heptanol; ○, *n*-hexanol; □, isoamyl alcohol; ☆, isooctyl alcohol; ▼, acetone; ◀, 1-butanone; ►, DMF; ◆, DMSO; △, acetonitrile; ▽, ethyl acetate; ◁, toluene; ▷, dioxane. —, calculated values via modified Apelblat equation.



**Figure S4.** Evaluated mixing Gibbs energy at measured solubility points based on the Wilson model: ●, toluene; ◆, acetonitrile; ★, ethyl acetate; ★, 1,4-dioxane; ◀, acetone; ▶, *n*-butanol; ■, methanol; ▼, isopropanol; ▲, *n*-propanol; □, ethanol; ○, isoamyl alcohol; △, *n*-hexanol; ▽, *n*-heptanol; ◇, isooctyl alcohol; ☆, DMF; ◁, DMSO.

**Table S1** Detailed Information on the Materials Used in this Work.

Chemicals	Molar mass $\text{g}\cdot\text{mol}^{-1}$	Melting point K	Melting Enthalpy $\text{KJ}\cdot\text{mol}^{-1}$	Density (293 K) $\text{kg}\cdot\text{m}^{-3}$	Source	Initial mass fraction purity	Final mass fraction purity	Purification method	Analytical method
1-Hydroxybenzotriazole	135.12	424.26 <sup>a</sup> 409.15 <sup>b</sup> 428-430 <sup>c</sup> 433 <sup>d</sup> 383 <sup>e</sup>	20.05 <sup>a</sup>	1510 <sup>f</sup>	Beijing HWRK Chemical Co., Ltd	0.980	0.992	Recrystallization	HPLC <sup>h</sup>
Methanol	32.04			786.5 <sup>g</sup>			0.995	---	GC <sup>i</sup>
Ethanol	46.07			789.3 <sup>g</sup>			0.997	---	GC
<i>n</i> -Propanol	60.10			805.3 <sup>g</sup>	Sinopharm		0.995	---	GC
Isopropanol	60.10			803.5 <sup>g</sup>	Chemical Reagent		0.997	---	GC
Ethyl acetate	88.11			900.3 <sup>g</sup>	Co., Ltd., China		0.995	---	GC
Acetonitrile	41.05			776.8 <sup>g</sup>			0.993	---	GC
Toluene	92.14			871.0 <sup>g</sup>			0.995	---	GC
1,4-dioxane	88.11			1033.7 <sup>g</sup>			0.995	---	GC
Acetone	58.05			784.5 <sup>g</sup>			0.995	---	GC
2-Butanone	72.11			801.4 <sup>g</sup>			0.995	---	GC
Isoamyl alcohol	88.15			813.0 <sup>g</sup>			0.994		GC
<i>n</i> -Hexanol	102.18			815.3 <sup>g</sup>			0.995		GC
<i>n</i> -Heptanol	116.20			821.9 <sup>g</sup>			0.993		GC
Isooctyl alcohol	130.23			834.4 <sup>g</sup>			0.993		GC
DMF	73.09			944.5 <sup>g</sup>			0.994		GC
DMSO	78.13			1100 <sup>g</sup>			0.993		GC

<sup>a</sup> This work, determined at 101.1 kPa. The standard uncertainties  $u$  are  $u(T) = 0.5$  K,  $u(p) = 0.45$  kPa,  $u(\Delta_{\text{fus}}H) = 0.4$  kJ·mol<sup>-1</sup>.

<sup>b,c,d,e</sup> Taken from References 1, 2, 3 and 4, respectively.

<sup>f</sup> Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs).

<sup>g</sup> Taken from Reference 5.

<sup>h</sup> High-performance liquid phase chromatograph.

<sup>i</sup> Gas chromatography.

**Table S2** Solubility parameters for the selected solvents.<sup>a</sup>

Compound	methanol	ethanol	<i>n</i> -propanol	isopropanol	2-butanone	acetone	ethyl acetate	acetonitrile
Solubility parameter (J·cm <sup>-3</sup> ) <sup>0.5</sup>	29.520	26.577	24.832	23.322	19.019	20.054	18.350	24.087
Compound	toluene	1,4-dioxane	isoamyl alcohol	<i>n</i> -hexanol	<i>n</i> -heptanol	isooctyl alcohol	DMF	DMSO
Solubility parameter (J·cm <sup>-3</sup> ) <sup>0.5</sup>	18.347	20.523	22.121	21.491	21.544	18.025	23.967	26.333

<sup>a</sup>Taken from Reference 6..

**Table S3** Parameters of the Equations and *RMSD* Values for HOBT in Different Solvents.

Solvent	Modified Apelblat equation				$\lambda h$ equation		
	<i>A</i>	<i>B</i>	<i>C</i>	$10^4 RMSD$	$\lambda$	<i>h</i>	$10^4 RMSD$
methanol	-219.68	7437.6	33.61	1.50	0.3899	6055.4	7.02
ethanol	-164.79	5152.1	25.37	1.61	0.4578	4837.0	7.06
<i>n</i> -propanol	-115.83	3029.8	18.02	0.96	0.3968	5390.3	4.25
isopropanol	-140.38	4043.7	21.70	0.98	0.3565	6196.9	4.45
2-butanone	-143.47	4037.6	22.18	0.56	0.2721	8629.3	2.95
acetone	-126.92	3281.2	19.70	0.46	0.2444	9681.0	2.22
ethyl acetate	-490.75	18052.0	74.72	1.13	0.6750	5979.4	5.87
acetonitrile	-142.49	3541.4	21.98	0.10	0.0693	40324.4	0.46
toluene	-24.07	-3369.6	4.396	0.01	0.0032	1429584	0.01
1,4-dioxane	-343.62	12386.2	52.34	0.94	0.5415	6072.3	3.82
isoamylalcohol	-78.470	2122.25	11.78	0.26	-0.0035	127825	1.86
<i>n</i> -hexanol	-88.710	2461.65	13.39	0.44	-0.0015	109974	1.87
<i>n</i> -heptaol	-152.37	5236.92	22.94	0.33	-0.0009	102759	0.85
isooctyl alcohol	-140.11	4884.55	20.97	0.21	-0.0043	138461	0.91
DMF	-57.730	-669.320	10.12	3.94	0.8229	4356.97	6.15
DMSO	-100.89	1067.25	16.64	1.76	4357.9	4937.73	7.29



**Table S4** Parameters of the Wilson and NRTL Models for HOBT in Different Solvents.

Solvent	Wilson Model					NRTL Model					
	$a_{12}$	$b_{12} / \text{K}$	$a_{21}$	$b_{21} / \text{K}$	$10^4 \text{ RMSD}$	$a_{12}$	$b_{12} / \text{K}$	$a_{21}$	$b_{21} / \text{K}$	$\alpha$	$10^4 \text{ RMSD}$
methanol	-0.9140	-3.6959	770.68	-122441	7.93	47.834	92126.2	1.391	-140.87	0.2	6.94
ethanol	-0.4832	-121.44	1160.4	-217995	8.24	2.531	-1393.5	-4.508	2612.6	0.2	1.81
<i>n</i> -propanol	-0.0017	-174.54	663.25	-109100	5.21	-0.0402	-493.79	2.264	282.11	0.2	0.85
isopropanol	0.0055	-120.48	500.91	-81227.8	5.31	1.921	-1125.8	-2.176	1768.4	0.2	0.98
2-butanone	0.2242	-3.8527	39.093	-1360.0	3.47	0.0936	-570.88	1.934	638.30	0.2	0.49
acetone	0.1011	12.415	18.180	2880.6	2.66	2.525	-1202.8	-2.942	1933.9	0.2	0.45
ethyl acetate	-3.659	1436.0	772.13	247663	6.74	3.465	-1578.9	-11.780	5244.3	0.3	1.65
acetonitrile	0.2612	377.88	-1904.4	849173	0.52	0.5809	-626.75	0.5654	1511.2	0.3	0.09
toluene	0.2261	2067.0	105.15	19959	0.01	-1.803	-394.32	3.248	3813.5	0.3	0.007
1,4-dioxane	-2.224	802.96	39.581	2668.8	4.07	3.383	-1743.2	-8.833	4426.2	0.2	1.10
isoamyl alcohol	5.032	-916.30	1.8360	-545.76	0.28	0.00988	-563.71	5.836	-313.95	0.2	0.28
<i>n</i> -hexanol	4.6924	-1064.5	173.35	2553.2	0.38	0.9304	-842.64	3.333	424.18	0.2	0.51
<i>n</i> -heptaol	4.6213	-1021.8	268.85	-3647.2	1.90	$9.612 \times 10^{-5}$	-701.33	5.277	171.95	0.2	0.33
isooctyl alcohol	5.6647	-1257.6	928.84	-0.2139	1.43	1.266	-1071.0	2.389	1048.0	0.2	0.25
DMF	-6.1439	1449.7	1541.4	-290910	15.21	-5.325	1552.2	131.78	29285.2	0.47	15.19
DMSO	-6.5001	1587.7	621.62	-59522.3	15.84	-6.282	1904.2	26.569	4697.3	0.47	6.92

**Table S5** Experimental Mole Fraction Solubility ( $x$ ) of HOBT in Different Solvents at the Temperature Range from  $T = (278.15 \text{ To } 313.15) \text{ K}$  under 101.1 kPa.<sup>a</sup>

$T/\text{K}$	100 $x$	100 $RD$			
		Modified Apelblat equation	$\lambda h$ equation	Wilson model	NRTL model
<i>methanol</i>					
278.15	2.232	-0.77	2.92	2.68	2.22
280.65	2.388	-0.26	1.87	1.62	1.33
283.15	2.542	-0.42	0.43	0.16	0.04
285.65	2.739	0.49	0.29	0.04	0.05
288.15	2.935	0.70	-0.29	-0.53	-0.40
290.65	3.138	0.56	-0.99	-1.20	-0.99
293.15	3.363	0.53	-1.35	-1.52	-1.25
295.65	3.581	-0.28	-2.27	-2.39	-2.09
298.15	3.861	0.05	-1.83	-1.88	-1.59
300.65	4.152	0.00	-1.56	-1.54	-1.28
303.15	4.445	-0.62	-1.67	-1.55	-1.36
305.65	4.799	-0.49	-0.83	-0.61	-0.52
308.15	5.218	0.25	0.78	1.11	1.07
310.65	5.622	-0.02	1.55	2.01	1.79
313.15	6.093	0.20	2.95	3.54	3.12
100 $RAD$		0.38	1.44	1.49	1.27
<i>ethanol</i>					
278.15	3.181	1.25	3.88	3.77	0.92
280.65	3.311	-0.95	0.60	0.44	-1.12
283.15	3.553	-0.18	0.40	0.21	-0.22
285.65	3.771	-0.61	-0.78	-1.00	-0.55
288.15	4.057	0.24	-0.51	-0.73	0.37
290.65	4.327	0.14	-1.01	-1.22	0.31
293.15	4.621	0.10	-1.29	-1.47	0.29
295.65	4.928	-0.15	-1.62	-1.76	0.03
298.15	5.281	0.01	-1.36	-1.45	0.17
300.65	5.655	0.04	-1.09	-1.11	0.15
303.15	6.050	-0.09	-0.84	-0.77	-0.03
305.65	6.508	0.27	0.04	0.21	0.26
308.15	6.967	0.09	0.51	0.79	-0.00

310.65	7.457	-0.16	1.03	1.44	-0.34
313.15	8.017	-0.02	2.05	2.60	-0.28
100 RAD		0.29	1.13	1.26	0.34
<i>n-propanol</i>					
278.15	2.972	-0.40	1.31	1.39	-0.17
280.65	3.185	0.10	1.06	1.06	0.18
283.15	3.397	0.09	0.45	0.38	0.07
285.65	3.622	0.03	-0.10	-0.22	-0.05
288.15	3.871	0.18	-0.32	-0.47	0.07
290.65	4.124	-0.02	-0.77	-0.94	-0.12
293.15	4.402	-0.04	-0.93	-1.10	-0.12
295.65	4.721	0.39	-0.53	-0.69	0.35
298.15	5.018	-0.09	-0.95	-1.08	-0.09
300.65	5.352	-0.24	-0.95	-1.03	-0.20
303.15	5.731	0.00	-0.47	-0.48	0.06
305.65	6.119	-0.08	-0.21	-0.14	-0.01
308.15	6.553	0.13	0.42	0.59	0.19
310.65	6.976	-0.26	0.51	0.80	-0.26
313.15	7.490	0.19	1.52	1.94	0.10
100 RAD		0.15	0.70	0.82	0.14
<i>isopropanol</i>					
278.15	2.476	0.40	2.51	2.51	0.42
280.65	2.613	-0.68	0.53	0.46	-0.69
283.15	2.813	0.17	0.62	0.50	0.15
285.65	3.006	0.23	0.07	-0.08	0.20
288.15	3.199	-0.18	-0.80	-0.97	-0.20
290.65	3.415	-0.32	-1.26	-1.44	-0.33
293.15	3.672	0.21	-0.90	-1.07	0.22
295.65	3.920	-0.02	-1.18	-1.33	0.01
298.15	4.208	0.27	-0.82	-0.92	0.31
300.65	4.508	0.31	-0.58	-0.63	0.36
303.15	4.806	-0.17	-0.75	-0.73	-0.12
305.65	5.147	-0.23	-0.39	-0.28	-0.19
308.15	5.530	0.01	0.36	0.57	0.01
310.65	5.919	-0.17	0.79	1.12	-0.22
313.15	6.370	0.17	1.82	2.29	0.05
100 RAD		0.24	0.89	0.99	0.23
<i>2-butanone</i>					

278.15	1.574	-0.46	1.68	1.66	-0.13
280.65	1.694	-0.02	1.19	1.12	0.09
283.15	1.814	-0.14	0.31	0.20	-0.18
285.65	1.954	0.28	0.12	-0.02	0.16
288.15	2.105	0.66	0.05	-0.11	0.50
290.65	2.245	-0.00	-0.94	-1.1	-0.16
293.15	2.408	-0.14	-1.26	-1.41	-0.26
295.65	2.590	-0.04	-1.20	-1.33	-0.10
298.15	2.785	-0.00	-1.08	-1.18	-0.003
300.65	2.988	-0.22	-1.11	-1.15	-0.16
303.15	3.225	0.12	-0.45	-0.43	0.23
305.65	3.467	0.04	-0.12	-0.02	0.17
308.15	3.720	-0.26	0.09	0.29	-0.16
310.65	4.018	0.07	1.03	1.33	0.08
313.15	4.327	0.08	1.73	2.15	-0.07
100 RAD		0.17	0.82	0.90	0.16
<i>acetone</i>					
278.15	1.389	0.26	2.05	2.05	0.28
280.65	1.486	-0.11	0.91	0.86	-0.11
283.15	1.596	-0.11	0.26	0.16	-0.12
285.65	1.712	-0.27	-0.41	-0.54	-0.29
288.15	1.842	-0.14	-0.68	-0.82	-0.16
290.65	1.983	0.01	-0.79	-0.94	0.001
293.15	2.138	0.30	-0.65	-0.79	0.30
295.65	2.294	0.08	-0.90	-1.03	0.09
298.15	2.464	-0.05	-0.96	-1.05	-0.02
300.65	2.659	0.27	-0.47	-0.51	0.31
303.15	2.855	0.08	-0.40	-0.39	0.11
305.65	3.060	-0.31	-0.44	-0.35	-0.28
308.15	3.302	-0.04	0.28	0.45	-0.02
310.65	3.549	-0.17	0.66	0.94	-0.19
313.15	3.833	0.18	1.58	1.97	0.10
100 RAD		0.16	0.76	0.86	0.16
<i>ethyl acetate</i>					
278.15	0.5050	0.50	9.50	7.57	-0.52
280.65	0.5548	0.89	6.27	4.59	0.16
283.15	0.6062	0.21	2.50	1.19	-0.19
285.65	0.6763	1.24	0.94	-0.03	1.09

288.15	0.7449	0.68	-1.65	-2.38	0.68
290.65	0.8206	-0.39	-4.22	-4.56	-0.12
293.15	0.9077	-1.23	-6.01	-6.16	-0.90
295.65	1.009	-2.08	-7.24	-7.07	-1.58
298.15	1.152	-0.53	-5.39	-4.96	0.06
300.65	1.298	-0.64	-4.75	-4.08	-0.02
303.15	1.487	0.59	-2.22	-1.35	1.15
305.65	1.686	0.48	-0.61	0.45	0.89
308.15	1.928	0.94	1.98	3.19	1.03
310.65	2.194	0.63	4.19	5.54	0.19
313.15	2.474	-0.86	5.64	7.11	-2.12
100 RAD		0.79	4.21	4.02	0.71
<i>acetonitrile</i>					
278.15	0.2291	-0.17	1.90	1.76	0.13
280.65	0.2488	-0.25	0.93	0.80	-0.13
283.15	0.2707	-0.16	0.28	0.15	-0.17
285.65	0.2952	0.14	-0.01	-0.14	0.04
288.15	0.3221	0.46	-0.12	-0.24	0.33
290.65	0.3476	-0.33	-1.23	-1.33	-0.46
293.15	0.3805	0.28	-0.78	-0.86	0.18
295.65	0.4143	0.35	-0.76	-0.81	0.29
298.15	0.4491	-0.05	-1.08	-1.10	-0.05
300.65	0.4882	-0.17	-1.01	-1.00	-0.13
303.15	0.5309	-0.27	-0.82	-0.76	-0.18
305.65	0.5802	0.12	-0.03	0.08	0.22
308.15	0.6311	0.03	0.36	0.53	0.11
310.65	0.6854	-0.23	0.68	0.92	-0.22
313.15	0.7493	0.17	1.72	2.03	0.04
100 RAD		0.21	0.78	0.83	0.18
<i>toluene</i>					
278.15	0.001105	3.04	2.98	2.44	0.99
280.65	0.001203	-3.19	-3.36	-3.76	-4.64
283.15	0.001496	4.07	3.85	3.62	3.32
285.65	0.001605	-3.14	-3.42	-3.54	-3.39
288.15	0.001985	4.01	3.73	3.72	4.21
290.65	0.002167	-1.00	-1.29	-1.21	-0.43
293.15	0.002487	-0.87	-1.14	-1.00	-0.05
295.65	0.002849	-0.74	-0.96	-0.78	0.24

298.15	0.003256	-0.64	-0.81	-0.61	0.38
300.65	0.003615	-3.30	-3.41	-3.19	-2.33
303.15	0.004282	0.80	0.77	0.97	1.53
305.65	0.004871	0.98	1.04	1.20	1.36
308.15	0.005561	1.70	1.84	1.95	1.57
310.65	0.006199	0.22	0.46	0.50	-0.60
313.15	0.006923	-0.92	-0.59	-0.63	-2.66
100 RAD		1.91	1.98	1.94	1.85
<i>1,4-dioxane</i>					
288.15	1.452	0.12	2.99	2.60	-0.11
290.65	1.582	0.46	1.66	1.35	0.33
293.15	1.713	-0.07	-0.15	-0.38	-0.09
295.65	1.869	-0.07	-1.07	-1.22	-0.01
298.15	2.024	-1.05	-2.62	-2.68	-0.91
300.65	2.245	0.16	-1.57	-1.56	0.34
303.15	2.466	0.19	-1.38	-1.30	0.38
305.65	2.721	0.46	-0.60	-0.45	0.62
308.15	2.976	-0.33	-0.59	-0.36	-0.27
310.65	3.309	0.33	1.20	1.49	0.24
313.15	3.642	-0.20	2.08	2.43	-0.54
100 RAD		0.31	1.45	1.44	0.35
<i>isoamyl alcohol</i>					
278.15	1.092	-0.17	-1.34	-0.12	-0.13
280.65	1.135	-0.05	-0.66	-0.05	-0.06
283.15	1.182	0.23	0.11	0.20	0.20
285.65	1.228	0.25	0.55	0.21	0.21
288.15	1.275	0.19	0.81	0.15	0.15
290.65	1.321	-0.11	0.76	-0.14	-0.14
293.15	1.370	-0.34	0.68	-0.35	-0.34
295.65	1.426	-0.22	0.84	-0.20	-0.20
298.15	1.483	-0.20	0.78	-0.17	-0.16
300.65	1.549	0.23	1.00	0.28	0.29
303.15	1.609	0.10	0.51	0.15	0.16
305.65	1.673	0.05	-0.05	0.09	0.10
308.15	1.743	0.18	-0.60	0.20	0.20
310.65	1.810	-0.03	-1.69	-0.05	-0.06
313.15	1.882	-0.12	-2.90	-0.21	-0.24
100 RAD		0.16	0.89	0.17	0.18

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<i>n-hexanol</i>					
278.15	1.139	0.30	-0.84	1.27	0.18
280.65	1.182	-0.10	-0.73	0.41	-0.19
283.15	1.234	0.07	-0.11	0.20	0.01
285.65	1.289	0.27	0.48	0.10	0.25
288.15	1.340	-0.05	0.48	-0.44	-0.03
290.65	1.394	-0.32	0.45	-0.85	-0.27
293.15	1.452	-0.49	0.43	-1.09	-0.41
295.65	1.519	-0.25	0.72	-0.85	-0.15
298.15	1.589	-0.04	0.88	-0.57	0.07
300.65	1.660	0.01	0.76	-0.39	0.13
303.15	1.738	0.26	0.71	0.04	0.36
305.65	1.818	0.40	0.41	0.41	0.46
308.15	1.898	0.33	-0.28	0.62	0.33
310.65	1.976	-0.03	-1.45	0.58	-0.14
313.15	2.058	-0.38	-2.82	0.60	-0.61
100 RAD		0.22	0.77	0.56	0.24
<i>n-heptanol</i>					
278.15	1.188	-0.32	-0.58	1.69	-0.08
280.65	1.235	-0.20	-0.40	0.87	-0.14
283.15	1.290	0.29	0.17	0.59	0.23
285.65	1.342	0.26	0.25	-0.05	0.13
288.15	1.396	0.12	0.22	-0.64	-0.03
290.65	1.457	0.21	0.42	-0.85	0.08
293.15	1.519	0.10	0.40	-1.12	0.01
295.65	1.584	-0.09	0.28	-1.33	-0.12
298.15	1.653	-0.29	0.11	-1.41	-0.25
300.65	1.731	-0.23	0.15	-1.10	-0.13
303.15	1.818	0.04	0.32	-0.46	0.19
305.65	1.901	-0.20	-0.10	-0.23	-0.05
308.15	2.005	0.33	0.15	0.88	0.44
310.65	2.098	0.01	-0.58	1.24	-0.001
313.15	2.203	-0.04	-1.19	1.96	-0.26
100 RAD		0.18	0.36	0.96	0.14
<i>isooctyl alcohol</i>					
278.15	1.080	-0.05	-0.47	1.72	-0.04
280.65	1.115	0.02	-0.26	0.96	-0.002
283.15	1.153	0.14	0.01	0.39	0.11

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285.65	1.193	0.21	0.24	-0.07	0.18
288.15	1.232	-0.01	0.17	-0.69	-0.04
290.65	1.275	-0.11	0.20	-1.06	-0.13
293.15	1.319	-0.35	0.07	-1.44	-0.34
295.65	1.372	-0.13	0.36	-1.22	-0.1
298.15	1.428	0.07	0.57	-0.92	0.11
300.65	1.485	0.09	0.54	-0.67	0.15
303.15	1.543	-0.04	0.27	-0.48	0.02
305.65	1.610	0.16	0.24	0.15	0.22
308.15	1.677	0.12	-0.15	0.62	0.14
310.65	1.748	0.08	-0.68	1.18	0.04
313.15	1.819	-0.19	-1.61	1.58	-0.32
100 RAD		0.12	0.39	0.88	0.13
<i>DMF</i>					
278.15	4.124	-0.72	0.13	1.42	0.81
280.65	4.644	-0.04	0.41	1.17	1.07
283.15	5.220	0.57	0.71	0.99	1.24
285.65	5.865	1.25	1.14	1.02	1.47
288.15	6.456	0.004	-0.29	-0.74	-0.22
290.65	7.199	0.16	-0.26	-0.95	-0.47
293.15	7.942	-0.65	-1.13	-2.00	-1.63
295.65	8.843	-0.43	-0.91	-1.85	-1.65
298.15	9.800	-0.58	-1.01	-1.92	-1.91
300.65	10.90	-0.21	-0.55	-1.36	-1.52
303.15	12.13	0.24	0.03	-0.49	-0.78
305.65	13.43	0.30	0.27	0.11	-0.23
308.15	14.85	0.34	0.53	0.83	0.55
310.65	16.37	0.12	0.56	1.51	1.38
313.15	17.98	-0.29	0.42	2.07	2.24
100 RAD		0.39	0.56	1.23	1.14
<i>DMSO</i>					
278.15	3.369	0.26	1.74	2.91	0.59
280.65	3.770	0.04	0.85	1.53	0.43
283.15	4.213	-0.25	0.003	0.24	0.13
285.65	4.746	0.33	0.15	0.01	0.62
288.15	5.287	-0.13	-0.64	-1.1	0.01
290.65	5.918	-0.05	-0.77	-1.47	-0.09
293.15	6.639	0.33	-0.50	-1.35	0.08



295.65	7.377	-0.18	-1.03	-1.96	-0.64
298.15	8.205	-0.53	-1.31	-2.21	-1.16
300.65	9.205	0.05	-0.56	-1.32	-0.66
303.15	10.26	0.07	-0.30	-0.84	-0.64
305.65	11.43	0.02	-0.03	-0.16	-0.45
308.15	12.75	0.23	0.56	0.90	0.14
310.65	14.16	0.07	0.83	1.77	0.59
313.15	15.71	-0.14	1.12	2.79	1.29
100 RAD		0.17	0.69	1.37	0.50

<sup>a</sup>Standard uncertainties  $u$  are  $u(T) = 0.02$  K,  $u(p) = 0.45$  kPa; Relative standard uncertainty  $u_r$  is  $u_r(x) = 0.027$ .

**Table S6** The Calculated Values for  $\Delta_{\text{mix}}G$ ,  $\Delta_{\text{mix}}H$ ,  $\Delta_{\text{mix}}S$ ,  $\ln \gamma_1^\infty$ , and  $H_1^{E,\infty}$ :  $\Delta_{\text{mix}}G$ ,  $\Delta_{\text{mix}}H$  and  $\Delta_{\text{mix}}S$  Denote the Mixing Gibbs Free Energy, Mixing Enthalpy, and Mixing Entropy, Respectively;  $\gamma_1^\infty$  Denotes the Activity Coefficient at Infinitesimal Concentration, and  $H_1^{E,\infty}$  Denotes Reduced Excess Enthalpy.

$T/\text{K}$	$\Delta_{\text{mix}}G$ J·mol <sup>-1</sup>	$\Delta_{\text{mix}}H$ J·mol <sup>-1</sup>	$\Delta_{\text{mix}}S$ J·K <sup>-1</sup> ·mol <sup>-1</sup>	$\ln \gamma_1^\infty$	$H_1^{E,\infty}$ kJ·mol <sup>-1</sup>
<i>Methanol</i>					
278.15	-203.4	-0.67	0.729	0.860	
280.65	-215.7	-0.72	0.766	0.860	
283.15	-227.9	-0.76	0.802	0.860	
285.65	-242.9	-0.82	0.847	0.860	
288.15	-257.7	-0.88	0.891	0.860	
290.65	-272.8	-0.94	0.935	0.860	
293.15	-289.1	-1.00	0.983	0.860	
295.65	-304.9	-1.07	1.028	0.860	-0.030
298.15	-324.3	-1.15	1.084	0.861	
300.65	-344.1	-1.23	1.140	0.861	
303.15	-363.7	-1.31	1.196	0.861	
305.65	-386.5	-1.41	1.260	0.861	
308.15	-412.5	-1.53	1.334	0.861	
310.65	-437.1	-1.64	1.402	0.861	
313.15	-464.6	-1.77	1.478	0.861	
<i>Ethanol</i>					
278.15	-289.0	-31.49	0.926	0.507	
280.65	-300.0	-32.74	0.952	0.511	
283.15	-318.5	-35.08	1.001	0.515	
285.65	-335.3	-37.17	1.044	0.519	
288.15	-356.4	-39.92	1.098	0.523	
290.65	-376.2	-42.49	1.148	0.526	
293.15	-397.3	-45.29	1.201	0.530	-1.01
295.65	-418.9	-48.19	1.254	0.533	
298.15	-443.1	-51.51	1.313	0.537	
300.65	-468.1	-55.01	1.374	0.540	
303.15	-493.9	-58.69	1.436	0.543	
305.65	-522.8	-62.93	1.505	0.547	

308.15	-551.3	-67.14	1.571	0.550	
310.65	-580.8	-71.60	1.639	0.553	
313.15	-613.3	-76.66	1.714	0.556	
<i>n-Propanol</i>					
278.15	-271.7	-42.30	0.825	0.552	
280.65	-288.1	-45.26	0.865	0.558	
283.15	-304.4	-48.20	0.905	0.563	
285.65	-321.4	-51.31	0.946	0.569	
288.15	-339.8	-54.73	0.989	0.574	
290.65	-358.2	-58.20	1.032	0.579	
293.15	-378.0	-61.99	1.078	0.584	
295.65	-400.1	-66.33	1.129	0.589	-1.45
298.15	-420.5	-70.34	1.175	0.594	
300.65	-442.9	-74.83	1.224	0.599	
303.15	-467.5	-79.89	1.278	0.604	
305.65	-492.1	-85.04	1.332	0.609	
308.15	-518.9	-90.77	1.389	0.613	
310.65	-544.5	-96.30	1.443	0.618	
313.15	-574.3	-103.0	1.505	0.622	
<i>Isopropanol</i>					
278.15	-225.7	-24.32	0.724	0.752	
280.65	-236.8	-25.64	0.752	0.755	
283.15	-252.0	-27.55	0.793	0.759	
285.65	-266.7	-29.39	0.831	0.763	
288.15	-281.2	-31.23	0.867	0.767	
290.65	-297.1	-33.27	0.908	0.770	
293.15	-315.3	-35.70	0.954	0.774	
295.65	-332.8	-38.02	0.997	0.777	-1.00
298.15	-352.5	-40.71	1.046	0.781	
300.65	-372.6	-43.50	1.095	0.784	
303.15	-392.3	-46.25	1.142	0.787	
305.65	-414.1	-49.38	1.193	0.791	
308.15	-437.9	-52.88	1.249	0.794	
310.65	-461.5	-56.39	1.304	0.797	
313.15	-487.9	-60.44	1.365	0.800	
<i>2-Butanone</i>					
278.15	-143.8	-0.49	0.515	1.205	-0.032

280.65	-153.2	-0.53	0.544	1.205	
283.15	-162.6	-0.57	0.572	1.205	
285.65	-173.3	-0.61	0.605	1.205	
288.15	-184.6	-0.66	0.638	1.205	
290.65	-195.1	-0.70	0.669	1.205	
293.15	-207.0	-0.75	0.703	1.206	
295.65	-219.9	-0.80	0.741	1.206	
298.15	-233.4	-0.86	0.780	1.206	
300.65	-247.3	-0.92	0.820	1.206	
303.15	-263.0	-0.99	0.864	1.206	
305.65	-278.7	-1.06	0.908	1.206	
308.15	-294.8	-1.14	0.953	1.206	
310.65	-313.1	-1.22	1.004	1.206	
313.15	-331.6	-1.31	1.055	1.206	
<i>Acetone</i>					
278.15	-126.8	1.41	0.461	1.336	
280.65	-134.5	1.50	0.485	1.335	
283.15	-143.1	1.61	0.511	1.335	
285.65	-152.0	1.73	0.538	1.335	
288.15	-161.8	1.85	0.568	1.334	
290.65	-172.2	1.99	0.599	1.334	
293.15	-183.4	2.14	0.633	1.333	
295.65	-194.6	2.29	0.666	1.333	0.103
298.15	-206.5	2.46	0.701	1.333	
300.65	-219.7	2.64	0.739	1.332	
303.15	-232.8	2.83	0.777	1.332	
305.65	-246.3	3.03	0.816	1.332	
308.15	-261.6	3.25	0.859	1.331	
310.65	-276.9	3.48	0.903	1.331	
313.15	-294.0	3.75	0.951	1.331	
<i>Ethyl acetate</i>					
278.15	-45.42	59.06	0.376	2.415	
280.65	-49.73	64.82	0.408	2.369	
283.15	-54.21	70.75	0.441	2.323	11.94
285.65	-59.98	78.82	0.486	2.279	
288.15	-65.71	86.70	0.529	2.235	
290.65	-71.96	95.37	0.576	2.192	

293.15	-79.00	105.3	0.629	2.15
295.65	-86.99	116.9	0.689	2.109
298.15	-97.58	133.0	0.773	2.068
300.65	-108.3	149.5	0.858	2.028
303.15	-121.6	170.6	0.964	1.989
305.65	-135.4	192.8	1.073	1.950
308.15	-151.4	219.5	1.203	1.912
310.65	-168.6	248.6	1.343	1.874
313.15	-186.4	279.0	1.486	1.838

*Acetonitrile*

278.15	-20.92	7.06	0.101	3.146
280.65	-22.53	7.66	0.108	3.134
283.15	-24.27	8.32	0.115	3.122
285.65	-26.19	9.05	0.123	3.111
288.15	-28.25	9.86	0.132	3.099
290.65	-30.22	10.62	0.141	3.088
293.15	-32.65	11.60	0.151	3.077
295.65	-35.12	12.60	0.161	3.066
298.15	-37.63	13.63	0.172	3.055
300.65	-40.39	14.78	0.183	3.045
303.15	-43.34	16.03	0.196	3.034
305.65	-46.63	17.46	0.210	3.024
308.15	-49.98	18.93	0.224	3.014
310.65	-53.49	20.48	0.238	3.004
313.15	-57.47	22.30	0.255	2.995

3.14

*Toluene*

278.15	-0.10	0.19	0.001	8.490
280.65	-0.11	0.20	0.001	8.424
283.15	-0.13	0.25	0.001	8.359
285.65	-0.14	0.27	0.001	8.295
288.15	-0.17	0.33	0.002	8.232
290.65	-0.19	0.36	0.002	8.170
293.15	-0.21	0.41	0.002	8.110
295.65	-0.24	0.47	0.002	8.05
298.15	-0.27	0.54	0.003	7.991
300.65	-0.30	0.60	0.003	7.934
303.15	-0.35	0.71	0.003	7.877
305.65	-0.39	0.80	0.004	7.821

17.18

308.15	-0.44	0.91	0.004	7.766	
310.65	-0.48	1.01	0.005	7.713	
313.15	-0.54	1.13	0.005	7.659	
<i>1,4-Dioxane</i>					
288.15	-126.4	94.40	0.766	1.611	
290.65	-136.5	102.6	0.823	1.587	
293.15	-146.8	111.0	0.879	1.564	
295.65	-158.6	120.8	0.945	1.540	
298.15	-170.4	130.6	1.009	1.518	
300.65	-186.0	144.4	1.099	1.495	6.68
303.15	-201.6	158.2	1.187	1.473	
305.65	-219.0	174.0	1.286	1.452	
308.15	-236.4	189.7	1.383	1.430	
310.65	-257.7	210.1	1.506	1.409	
313.15	-278.9	230.3	1.626	1.389	
<i>Isoamyl alcohol</i>					
278.15	-99.61	-125.0	-0.091	1.609	
280.65	-102.3	-128.8	-0.095	1.655	
283.15	-105.2	-133.0	-0.098	1.699	
285.65	-107.9	-137.0	-0.102	1.743	
288.15	-110.7	-141.0	-0.105	1.785	
290.65	-113.4	-144.8	-0.108	1.827	
293.15	-116.2	-148.9	-0.112	1.867	
295.65	-119.3	-153.7	-0.116	1.907	-11.43
298.15	-122.4	-158.4	-0.121	1.946	
300.65	-126.0	-163.9	-0.126	1.984	
303.15	-129.1	-168.8	-0.131	2.021	
305.65	-132.4	-173.9	-0.136	2.057	
308.15	-135.9	-179.5	-0.142	2.093	
310.65	-139.1	-184.6	-0.147	2.128	
313.15	-142.5	-190.2	-0.152	2.162	
<i>n-hexanol</i>					
278.15	-104.2	-98.9	0.019	1.529	
280.65	-107.1	-102.5	0.017	1.563	
283.15	-110.6	-106.8	0.014	1.596	-8.85
285.65	-114.3	-111.3	0.010	1.629	
288.15	-117.6	-115.5	0.007	1.661	
290.65	-121.1	-120.0	0.004	1.693	

293.15	-124.7	-124.7	-0.000	1.724	
295.65	-128.8	-130.2	-0.005	1.755	
298.15	-133.0	-135.8	-0.010	1.785	
300.65	-137.1	-141.5	-0.015	1.815	
303.15	-141.5	-147.7	-0.020	1.844	
305.65	-146.0	-154.1	-0.026	1.873	
308.15	-150.3	-160.3	-0.033	1.901	
310.65	-154.4	-166.4	-0.039	1.929	
313.15	-158.6	-172.7	-0.045	1.956	
<i>n-heptaol</i>					
278.15	-108.5	-99.0	0.034	1.490	
280.65	-111.8	-102.7	0.032	1.523	
283.15	-115.5	-107.2	0.03	1.555	
285.65	-119.0	-111.3	0.027	1.587	
288.15	-122.6	-115.6	0.024	1.618	
290.65	-126.5	-120.4	0.021	1.648	
293.15	-130.4	-125.2	0.018	1.678	
295.65	-134.5	-130.3	0.014	1.708	-8.50
298.15	-138.6	-135.7	0.010	1.737	
300.65	-143.3	-141.7	0.005	1.765	
303.15	-148.3	-148.4	-0.000	1.793	
305.65	-152.9	-154.7	-0.006	1.821	
308.15	-158.6	-162.6	-0.013	1.848	
310.65	-163.6	-169.5	-0.019	1.875	
313.15	-169.0	-177.3	-0.027	1.901	
<i>isooctyl alcohol</i>					
278.15	-98.60	-110.7	-0.044	1.587	
280.65	-100.9	-114.2	-0.047	1.627	
283.15	-103.3	-117.9	-0.051	1.667	-10.45
285.65	-105.8	-121.8	-0.056	1.706	
288.15	-108.2	-125.5	-0.060	1.744	
290.65	-110.8	-129.7	-0.065	1.782	
293.15	-113.4	-133.9	-0.070	1.818	
295.65	-116.4	-138.9	-0.076	1.855	
298.15	-119.6	-144.2	-0.083	1.89	
300.65	-122.7	-149.6	-0.089	1.925	
303.15	-125.8	-155.0	-0.096	1.960	
305.65	-129.4	-161.2	-0.104	1.994	

308.15	-132.8	-167.4	-0.112	2.027	
310.65	-136.3	-173.8	-0.121	2.060	
313.15	-139.7	-180.2	-0.129	2.092	
<i>DMF</i>					
278.15	-376.9	487.5	3.108	0.213	
280.65	-420	548.1	3.45	0.167	
283.15	-467	615.1	3.822	0.121	
285.65	-518.7	689.8	4.231	0.076	
288.15	-567.1	758.2	4.6	0.032	
290.65	-625.4	843.9	5.055	-0.011	
293.15	-683.9	929.3	5.503	-0.053	
295.65	-752.1	1032.3	6.036	-0.095	12.05
298.15	-823.6	1141.4	6.59	-0.136	
300.65	-903.1	1266	7.215	-0.177	
303.15	-989.6	1404.6	7.897	-0.217	
305.65	-1079.2	1550.2	8.603	-0.256	
308.15	-1174.5	1708.2	9.355	-0.294	
310.65	-1274.0	1876.1	10.14	-0.332	
313.15	-1376.8	2052.7	10.951	-0.369	
<i>DMSO</i>					
278.15	-306.7	436.0	2.670	0.439	
280.65	-340.7	487.3	2.950	0.388	
283.15	-377.7	543.8	3.254	0.338	
285.65	-420.9	611.5	3.614	0.289	
288.15	-464.9	680.1	3.974	0.241	
290.65	-514.9	759.8	4.386	0.194	
293.15	-570.6	850.6	4.848	0.147	
295.65	-627.6	943.2	5.313	0.101	13.20
298.15	-690.1	1046.7	5.825	0.056	
300.65	-762.5	1170.9	6.431	0.012	
303.15	-837.9	1301.3	7.057	-0.032	
305.65	-919.4	1445.1	7.736	-0.075	
308.15	-1008.3	1606.2	8.484	-0.117	
310.65	-1101.1	1777.1	9.265	-0.158	
313.15	-1199.9	1963.4	10.102	-0.199	

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