Solubility Data of the Bioactive Compound Piperine in (Transcutol + Water) Mixtures: Computational Modeling, Hansen Solubility Parameters and Mixing Thermodynamic Parameters

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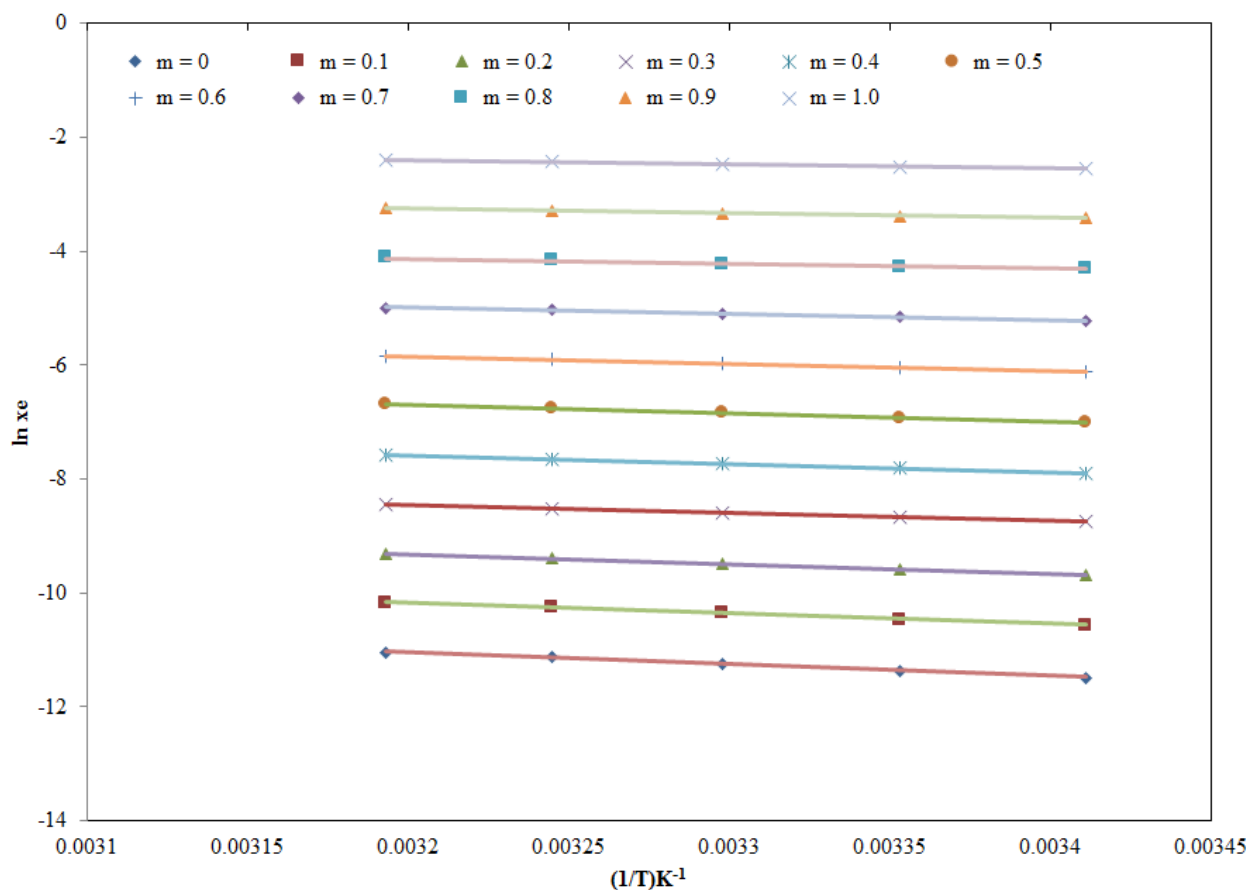
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Figure S1. Correlation of experimental solubility values of PPN with Van't Hoff model in different THP + water mixtures at T = 298.2 K to 318.2 K; Van't Hoff model solubility values of PPN are represented by solid lines, and experimental solubility values of PPN are represented by the symbols.

Table S1. Hansen solubility parameters (δ_{mix}/MPa$^{1/2}$) for various THP + water mixtures free of

PPN at $T = 298.2$ K

m	δ_{mix}/MPa$^{1/2}$
0.1	45.16
0.2	42.52
0.3	39.88
0.4	37.24
0.5	34.60
0.6	31.96
0.7	29.32
0.8	26.68
0.9	24.04

Table S2. The values of mixing enthalpy ($\Delta_{mix}H$/J mol^{-1}), mixing entropy ($\Delta_{mix}S$/J mol^{-1} K^{-1}), mixing Gibbs energy ($\Delta_{mix}G$/J mol^{-1}) and activity coefficient (γ_i) for PPN dissolution in different THP + water mixtures[a].

T/K	$\Delta_{mix}H$/J mol^{-1}	$\Delta_{mix}G$/J mol^{-1}	$\Delta_{mix}S$/J mol^{-1} K^{-1}	γ_i
$m = 0.0$				
298.2	−1170	774	−6.52	4980
303.2	−1200	791	−6.55	5150
308.2	−1220.	811	−6.60	5380
313.2	−1250	830	−6.63	5620
318.2	−1280	854	−6.70	6050
$m = 0.1$				
298.2	−955	571	−5.12	1995
303.2	−978	587	−5.16	2108
308.2	−1000	603	−5.20	2215
313.2	−1020	620	−5.25	2329
318.2	−1050	641	−5.32	2533
$m = 0.2$				
298.2	−764	397	−3.89	827
303.2	−784	411	−3.94	875
308.2	−803	424	−3.98	927
313.2	−824	438	−4.02	984
318.2	−847	455	−4.09	1070
$m = 0.3$				
298.2	−589	242	−2.78	322
303.2	−608	255	−2.84	353
308.2	−626	267	−2.89	380
313.2	−646	281	−2.96	416
318.2	−665	294	−3.01	448
$m = 0.4$				
298.2	−443	119	−1.88	138
303.2	−457	128	−1.93	148
308.2	−472	137	−1.97	160
313.2	−487	146	−2.02	173
318.2	−503	157	−2.07	189
$m = 0.5$				
298.2	−316	16	−1.11	56
303.2	−328	23	−1.15	61
308.2	−338	28	−1.19	65
313.2	−351	36	−1.23	71
318.2	−363	43	−1.27	77
$m = 0.6$				
298.2	−208	−63	−0.48	23
303.2	−217	−58	−0.52	25
308.2	−227	−52	−0.56	27
313.2	−237	−47	−0.60	30
318.2	−248	−41	−0.65	33
$m = 0.7$				
298.2	−123	−117	−0.02	9
303.2	−131	−114	−0.05	10
308.2	−138	−110	−0.09	11
313.2	−146	−107	−0.12	12
318.2	−155	−102	−0.16	14

m = 0.8				
298.2	−57	−147	0.30	3
303.2	−63	−144	0.26	4
308.2	−70	−142	0.23	5
313.2	−75	−140	0.20	5
318.2	−81	−137	0.17	6
m = 0.9				
298.2	−14	−149	0.45	1.57
303.2	−18	−147	0.42	1.79
308.2	−22	−146	0.40	2.00
313.2	−26	−145	0.37	2.23
318.2	−30	−144	0.35	2.49
m = 1.0				
298.2	8	−111	0.40	0.65
303.2	6	−110	0.38	0.74
308.2	4	−110	0.36	0.83
313.2	1	−110	0.35	0.94
318.2	1	−110	0.34	1.06

[a]The average relative uncertainties are $u(\Delta_{mix}H) = 0.90$, $u(\Delta_{mix}G) = 2.04$ and $u(\Delta_{mix}S) = 1.19$.