

Supporting Information

Liquid-Liquid Equilibria for Ternary System Water + Benzyl Alcohol + Methylbenzene at (303.2 to 343.2) K

Hui Wang¹, Qinbo Wang^{1*}, Zhenhua Xiong², Chuxiong Chen²

1. *Department of Chemical Engineering, Hunan University, Changsha, 410082 Hunan, P.R.China*
2. *Zhejiang Shuyang Chemical Co.Ltd., Quzhou, 324002 Zhejiang, P.R.China*

* To whom correspondence should be addressed. E-mail: qinbowang@126.com;

Table A. Experimental Deviations for Liquid-Liquid Equilibrium Data of Ternary Water (1) + Benzyl Alcohol (2) + Toluene (3) System at (303.2 to 343.2) K.

aqueous phase			organic phase		
w_1	w_2	w_3	w_1	w_2	w_3
$T=303.2\text{K}$					
0.0300	0.0000	0.0000	0.0000	0.0000	0.0300
0.0295	0.0005	0.0000	0.0001	0.0031	0.0267
0.0293	0.0006	0.0001	0.0003	0.0061	0.0237
0.0293	0.0006	0.0001	0.0005	0.0089	0.0207
0.0292	0.0007	0.0001	0.0006	0.0112	0.0182
0.0291	0.0008	0.0001	0.0008	0.0135	0.0157
0.0291	0.0008	0.0001	0.0010	0.0155	0.0135
0.0290	0.0009	0.0000	0.0012	0.0172	0.0116
0.0290	0.0010	0.0000	0.0013	0.0186	0.0101
0.0290	0.0010	0.0000	0.0014	0.0202	0.0084
0.0289	0.0010	0.0000	0.0016	0.0212	0.0073
0.0287	0.0013	0.0000	0.0031	0.0269	0.0000
$T=313.2\text{K}$					
0.0299	0.0000	0.0001	0.0002	0.0000	0.0298
0.0294	0.0005	0.0001	0.0001	0.0037	0.0262
0.0293	0.0006	0.0001	0.0003	0.0058	0.0238
0.0293	0.0007	0.0001	0.0005	0.0086	0.0209
0.0292	0.0008	0.0001	0.0007	0.0111	0.0182
0.0291	0.0008	0.0001	0.0009	0.0126	0.0165
0.0290	0.0009	0.0001	0.0010	0.0155	0.0135
0.0290	0.0010	0.0001	0.0012	0.0171	0.0116
0.0289	0.0010	0.0000	0.0013	0.0186	0.0101
0.0289	0.0011	0.0000	0.0015	0.0198	0.0087
0.0289	0.0011	0.0000	0.0017	0.0211	0.0073

0.0286	0.0014	0.0000	0.0032	0.0268	0.0000
$T=323.2\text{K}$					
0.0300	0.0000	0.0000	0.0000	0.0000	0.0300
0.0294	0.0005	0.0001	0.0002	0.0030	0.0268
0.0293	0.0006	0.0001	0.0004	0.0061	0.0235
0.0292	0.0007	0.0001	0.0005	0.0086	0.0209
0.0292	0.0008	0.0001	0.0008	0.0112	0.0180
0.0291	0.0008	0.0001	0.0009	0.0133	0.0158
0.0290	0.0009	0.0001	0.0011	0.0153	0.0136
0.0290	0.0010	0.0001	0.0013	0.0166	0.0121
0.0289	0.0011	0.0001	0.0014	0.0182	0.0104
0.0289	0.0011	0.0000	0.0016	0.0197	0.0087
0.0288	0.0011	0.0000	0.0018	0.0210	0.0072
0.0286	0.0014	0.0000	0.0034	0.0266	0.0000
$T=333.2\text{K}$					
0.0299	0.0000	0.0001	0.0001	0.0000	0.0299
0.0294	0.0005	0.0001	0.0001	0.0031	0.0268
0.0293	0.0006	0.0001	0.0003	0.0058	0.0239
0.0292	0.0007	0.0001	0.0005	0.0085	0.0209
0.0291	0.0008	0.0001	0.0008	0.0112	0.0180
0.0290	0.0009	0.0001	0.0010	0.0132	0.0159
0.0289	0.0010	0.0000	0.0012	0.0155	0.0133
0.0289	0.0011	0.0000	0.0013	0.0170	0.0116
0.0288	0.0012	0.0001	0.0016	0.0187	0.0097
0.0287	0.0012	0.0001	0.0018	0.0197	0.0085
0.0287	0.0012	0.0001	0.0020	0.0210	0.0070
0.0285	0.0015	0.0000	0.0037	0.0263	0.0000
$T=343.2\text{K}$					

0.0299	0.0000	0.0001	0.0001	0.0000	0.0299
0.0294	0.0005	0.0001	0.0002	0.0031	0.0266
0.0293	0.0006	0.0001	0.0005	0.0062	0.0233
0.0291	0.0008	0.0001	0.0007	0.0089	0.0203
0.0291	0.0008	0.0001	0.0009	0.0114	0.0177
0.0290	0.0009	0.0001	0.0011	0.0135	0.0154
0.0290	0.0010	0.0000	0.0014	0.0159	0.0127
0.0289	0.0010	0.0001	0.0014	0.0172	0.0114
0.0288	0.0011	0.0001	0.0017	0.0190	0.0093
0.0288	0.0012	0.0001	0.0018	0.0203	0.0079
0.0287	0.0013	0.0001	0.0021	0.0208	0.0071
0.0285	0.0015	0.0000	0.0042	0.0258	0.0000

Table B. The calculated G_{ij} for NRTL model using the regressed model parameters for Binary Water (1) + Toluene (3) System at (288.2 to 323.2) K.

T/K	G_{ij}^a			T/K	G_{ij}^b		
		$j=1$	$j=3$			$j=1$	$j=3$
303.2	$i=1$	1.000	0.223	288.2	$i=1$	1.000	0.339
	$i=3$	0.049	1.000		$i=3$	0.022	1.000
313.2	$i=1$	1.000	0.226	298.2	$i=1$	1.000	0.379
	$i=3$	0.052	1.000		$i=3$	0.022	1.000
323.2	$i=1$	1.000	0.228	313.2	$i=1$	1.000	0.437
	$i=3$	0.054	1.000		$i=3$	0.043	1.000

^a calculated by using the model parameters listed in Table 7.

^b calculated by using the model parameters reported in literature 12.