

Supporting Information

Liquid-liquid equilibria in the binary systems (1,3-dimethylimidazolium, or 1-butyl-3-methylimidazolium methylsulfate + hydrocarbons)^{†‡}

Urszula Domańska,^{1*} Aneta Pobudkowska¹ and Frank Eckert²

¹ *Physical Chemistry Division, Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland.*

² *COSMOlogic GmbH&Co. KG, Burscheider Str. 515, D-51381 Leverkusen, Germany.*

Keywords: Ionic liquids; Experimental (liquid + liquid) equilibria; Molecular interactions; COSMO-RS prediction

* Author to whom correspondence should be addressed: E-mail: ula@ch.pw.edu.pl

† Presented at the 1st International Congress on Ionic Liquids (COIL), Salzburg, Austria, June 19-22, 2005.

TABLE 1S: Liquid–Liquid Phase Equilibria Predicted by the COSMO-RS for $\{x_1$ [mmim][CH₃SO₄] + (1- x_1) Hydrocarbon} Mixtures

| T (K) | x_1' | x_1'' | T (K) | x_1' | x_1'' |
|-------------------|---------|---------|---------|---------|---------|
| <i>n</i> -pentane | | | | | |
| 298.15 | 0.95283 | 0.00001 | 563.15 | 0.85162 | 0.01036 |
| 308.15 | 0.95252 | 0.00001 | 568.15 | 0.84748 | 0.01108 |
| 313.15 | 0.95225 | 0.00002 | 573.15 | 0.84323 | 0.01184 |
| 323.15 | 0.95148 | 0.00003 | 578.15 | 0.83886 | 0.01264 |
| 333.15 | 0.95042 | 0.00004 | 583.15 | 0.83436 | 0.01348 |
| 338.15 | 0.94979 | 0.00005 | 588.15 | 0.82975 | 0.01437 |
| 343.15 | 0.94910 | 0.00006 | 593.15 | 0.82501 | 0.01530 |
| 348.15 | 0.94834 | 0.00008 | 598.15 | 0.82014 | 0.01627 |
| 353.15 | 0.94752 | 0.00009 | 603.15 | 0.81513 | 0.01730 |
| 358.15 | 0.94663 | 0.00011 | 608.15 | 0.80999 | 0.01838 |
| 363.15 | 0.94569 | 0.00014 | 613.15 | 0.80470 | 0.01951 |
| 368.15 | 0.94468 | 0.00016 | 618.15 | 0.79927 | 0.02070 |
| 373.15 | 0.94361 | 0.00019 | 623.15 | 0.79370 | 0.02195 |
| 378.15 | 0.94248 | 0.00023 | 628.15 | 0.78797 | 0.02326 |
| 383.15 | 0.94129 | 0.00027 | 633.15 | 0.78208 | 0.02463 |
| 388.15 | 0.94004 | 0.00032 | 638.15 | 0.77603 | 0.02607 |
| 393.15 | 0.93873 | 0.00037 | 643.15 | 0.76981 | 0.02758 |
| 398.15 | 0.93736 | 0.00042 | 648.15 | 0.76342 | 0.02917 |
| 403.15 | 0.93593 | 0.00049 | 653.15 | 0.75685 | 0.03083 |
| 408.15 | 0.93443 | 0.00056 | 658.15 | 0.75010 | 0.03258 |
| 413.15 | 0.93287 | 0.00064 | 663.15 | 0.74316 | 0.03441 |
| 418.15 | 0.93125 | 0.00073 | 668.15 | 0.73603 | 0.03633 |
| 423.15 | 0.92957 | 0.00083 | 673.15 | 0.72869 | 0.03835 |
| 428.15 | 0.92782 | 0.00093 | 678.15 | 0.72114 | 0.04047 |
| 433.15 | 0.92601 | 0.00105 | 683.15 | 0.71337 | 0.04270 |
| 438.15 | 0.92413 | 0.00118 | 688.15 | 0.70537 | 0.04504 |
| 443.15 | 0.92219 | 0.00132 | 693.15 | 0.69714 | 0.04750 |
| 448.15 | 0.92017 | 0.00148 | 698.15 | 0.68865 | 0.05009 |
| 453.15 | 0.91809 | 0.00164 | 703.15 | 0.67991 | 0.05281 |
| 458.15 | 0.91594 | 0.00182 | 708.15 | 0.67089 | 0.05568 |
| 463.15 | 0.91371 | 0.00202 | 713.15 | 0.66158 | 0.05870 |
| 468.15 | 0.91141 | 0.00223 | 718.15 | 0.65196 | 0.06193 |
| 473.15 | 0.90904 | 0.00246 | 723.15 | 0.64201 | 0.06530 |
| 478.15 | 0.90659 | 0.00270 | 728.15 | 0.63172 | 0.06886 |
| 483.15 | 0.90406 | 0.00296 | 733.15 | 0.62106 | 0.07264 |
| 488.15 | 0.90146 | 0.00324 | 738.15 | 0.60999 | 0.07664 |
| 493.15 | 0.89877 | 0.00354 | 743.15 | 0.59848 | 0.08088 |
| 498.15 | 0.89600 | 0.00386 | 748.15 | 0.58649 | 0.08540 |
| 503.15 | 0.89315 | 0.00420 | 753.15 | 0.57397 | 0.09021 |
| 508.15 | 0.89021 | 0.00457 | 758.15 | 0.56086 | 0.09535 |
| 513.15 | 0.88718 | 0.00495 | 763.15 | 0.54717 | 0.10075 |
| 518.15 | 0.88406 | 0.00537 | 768.15 | 0.53228 | 0.10666 |
| 523.15 | 0.88086 | 0.00580 | 773.15 | 0.51673 | 0.11300 |
| 528.15 | 0.87755 | 0.00627 | 778.15 | 0.50052 | 0.11968 |
| 533.15 | 0.87415 | 0.00676 | 783.15 | 0.48189 | 0.12742 |
| 538.15 | 0.87065 | 0.00728 | 788.15 | 0.46294 | 0.13533 |
| 543.15 | 0.86706 | 0.00783 | 793.15 | 0.44006 | 0.14426 |
| 548.15 | 0.86336 | 0.00841 | 798.15 | 0.41170 | 0.15424 |
| 553.15 | 0.85955 | 0.00903 | 803.15 | 0.34657 | 0.16744 |
| 558.15 | 0.85564 | 0.00968 | | | |
| cyclohexane | | | | | |
| 303.15 | 0.95061 | 0.00001 | 558.15 | 0.84677 | 0.00889 |
| 313.15 | 0.94995 | 0.00001 | 568.15 | 0.83822 | 0.01020 |
| 318.15 | 0.94950 | 0.00002 | 573.15 | 0.83377 | 0.01091 |
| 328.15 | 0.94840 | 0.00003 | 583.15 | 0.82451 | 0.01245 |

| | | | | | |
|--------------|---------|---------|--------|---------|---------|
| 338.15 | 0.94702 | 0.00004 | 593.15 | 0.81474 | 0.01415 |
| 348.15 | 0.94537 | 0.00006 | 598.15 | 0.80965 | 0.01507 |
| 353.15 | 0.94445 | 0.00008 | 608.15 | 0.79908 | 0.01705 |
| 358.15 | 0.94347 | 0.00010 | 613.15 | 0.79358 | 0.01812 |
| 363.15 | 0.94242 | 0.00012 | 623.15 | 0.78215 | 0.02042 |
| 368.15 | 0.94132 | 0.00014 | 628.15 | 0.77620 | 0.02165 |
| 373.15 | 0.94014 | 0.00017 | 638.15 | 0.76382 | 0.02431 |
| 378.15 | 0.93891 | 0.00020 | 643.15 | 0.75739 | 0.02575 |
| 383.15 | 0.93762 | 0.00023 | 653.15 | 0.74400 | 0.02883 |
| 388.15 | 0.93626 | 0.00027 | 658.15 | 0.73703 | 0.03051 |
| 393.15 | 0.93484 | 0.00032 | 668.15 | 0.72252 | 0.03409 |
| 398.15 | 0.93336 | 0.00037 | 673.15 | 0.71497 | 0.03601 |
| 408.15 | 0.93020 | 0.00049 | 683.15 | 0.69923 | 0.04013 |
| 418.15 | 0.92679 | 0.00064 | 688.15 | 0.69103 | 0.04236 |
| 428.15 | 0.92311 | 0.00082 | 698.15 | 0.67390 | 0.04719 |
| 438.15 | 0.91916 | 0.00104 | 703.15 | 0.66496 | 0.04979 |
| 448.15 | 0.91493 | 0.00131 | 713.15 | 0.64626 | 0.05544 |
| 458.15 | 0.91042 | 0.00162 | 718.15 | 0.63647 | 0.05851 |
| 468.15 | 0.90561 | 0.00199 | 728.15 | 0.61590 | 0.06519 |
| 473.15 | 0.90309 | 0.00220 | 733.15 | 0.60509 | 0.06882 |
| 478.15 | 0.90049 | 0.00242 | 743.15 | 0.58226 | 0.07677 |
| 488.15 | 0.89505 | 0.00292 | 748.15 | 0.57017 | 0.08114 |
| 493.15 | 0.89220 | 0.00319 | 753.15 | 0.55756 | 0.08565 |
| 503.15 | 0.88625 | 0.00380 | 763.15 | 0.53053 | 0.09626 |
| 508.15 | 0.88315 | 0.00414 | 768.15 | 0.51595 | 0.10205 |
| 513.15 | 0.87995 | 0.00449 | 778.15 | 0.48392 | 0.11495 |
| 523.15 | 0.87328 | 0.00528 | 783.15 | 0.46599 | 0.12236 |
| 528.15 | 0.86980 | 0.00571 | 788.15 | 0.44618 | 0.13049 |
| 538.15 | 0.86254 | 0.00665 | 793.15 | 0.42336 | 0.13950 |
| 543.15 | 0.85876 | 0.00717 | 803.15 | 0.34700 | 0.16173 |
| 553.15 | 0.85088 | 0.00829 | | | |
| cycloheptane | | | | | |
| 303.15 | 0.96969 | 0.00001 | 568.15 | 0.88879 | 0.01008 |
| 313.15 | 0.96925 | 0.00001 | 573.15 | 0.88546 | 0.01077 |
| 318.15 | 0.96896 | 0.00002 | 583.15 | 0.87850 | 0.01227 |
| 328.15 | 0.96821 | 0.00003 | 593.15 | 0.87113 | 0.01392 |
| 338.15 | 0.96728 | 0.00004 | 598.15 | 0.86729 | 0.01481 |
| 348.15 | 0.96616 | 0.00006 | 608.15 | 0.85927 | 0.01672 |
| 353.15 | 0.96553 | 0.00008 | 613.15 | 0.85509 | 0.01774 |
| 358.15 | 0.96485 | 0.00010 | 623.15 | 0.84636 | 0.01994 |
| 363.15 | 0.96414 | 0.00012 | 628.15 | 0.84181 | 0.02112 |
| 368.15 | 0.96337 | 0.00014 | 638.15 | 0.83232 | 0.02365 |
| 373.15 | 0.96257 | 0.00016 | 643.15 | 0.82737 | 0.02501 |
| 378.15 | 0.96171 | 0.00019 | 653.15 | 0.81704 | 0.02791 |
| 383.15 | 0.96082 | 0.00023 | 658.15 | 0.81165 | 0.02946 |
| 388.15 | 0.95988 | 0.00027 | 668.15 | 0.80041 | 0.03278 |
| 393.15 | 0.95889 | 0.00031 | 673.15 | 0.79455 | 0.03451 |
| 398.15 | 0.95786 | 0.00037 | 683.15 | 0.78231 | 0.03831 |
| 408.15 | 0.95565 | 0.00049 | 688.15 | 0.77592 | 0.04035 |
| 418.15 | 0.95326 | 0.00064 | 698.15 | 0.76257 | 0.04471 |
| 428.15 | 0.95067 | 0.00082 | 703.15 | 0.75559 | 0.04704 |
| 438.15 | 0.94788 | 0.00104 | 713.15 | 0.74100 | 0.05205 |
| 448.15 | 0.94488 | 0.00131 | 718.15 | 0.73336 | 0.05474 |
| 458.15 | 0.94167 | 0.00162 | 728.15 | 0.71736 | 0.06052 |
| 468.15 | 0.93823 | 0.00199 | 733.15 | 0.70897 | 0.06363 |
| 473.15 | 0.93642 | 0.00219 | 743.15 | 0.69133 | 0.07034 |
| 478.15 | 0.93455 | 0.00241 | 748.15 | 0.68206 | 0.07396 |
| 488.15 | 0.93062 | 0.00291 | 753.15 | 0.67245 | 0.07777 |
| 493.15 | 0.92856 | 0.00318 | 763.15 | 0.65213 | 0.08604 |
| 503.15 | 0.92424 | 0.00378 | 768.15 | 0.64138 | 0.09054 |

| | | | | | |
|---------|---------|---------|--------|---------|---------|
| 508.15 | 0.92198 | 0.00412 | 778.15 | 0.61846 | 0.10029 |
| 513.15 | 0.91965 | 0.00447 | 783.15 | 0.60621 | 0.10566 |
| 523.15 | 0.91476 | 0.00525 | 788.15 | 0.59335 | 0.11138 |
| 528.15 | 0.91221 | 0.00567 | 793.15 | 0.57978 | 0.11749 |
| 538.15 | 0.90686 | 0.00660 | 803.15 | 0.55006 | 0.13108 |
| 543.15 | 0.90406 | 0.00710 | 808.15 | 0.53349 | 0.13872 |
| 553.15 | 0.89822 | 0.00820 | 813.15 | 0.51545 | 0.14696 |
| 558.15 | 0.89517 | 0.00879 | 823.15 | 0.47203 | 0.16584 |
| benzene | | | | | |
| 253.15 | 0.65190 | 0.00030 | 398.15 | 0.59169 | 0.01273 |
| 258.15 | 0.65449 | 0.00037 | 403.15 | 0.58571 | 0.01387 |
| 263.15 | 0.65665 | 0.00044 | 408.15 | 0.57951 | 0.01508 |
| 268.15 | 0.65839 | 0.00053 | 413.15 | 0.57307 | 0.01638 |
| 273.15 | 0.65972 | 0.00063 | 418.15 | 0.56640 | 0.01776 |
| 278.15 | 0.66066 | 0.00075 | 423.15 | 0.55949 | 0.01923 |
| 283.15 | 0.66122 | 0.00088 | 428.15 | 0.55233 | 0.02080 |
| 288.15 | 0.66140 | 0.00103 | 433.15 | 0.54492 | 0.02249 |
| 293.15 | 0.66123 | 0.00120 | 438.15 | 0.53726 | 0.02427 |
| 298.15 | 0.66070 | 0.00139 | 443.15 | 0.52932 | 0.02617 |
| 303.15 | 0.65986 | 0.00160 | 448.15 | 0.52111 | 0.02820 |
| 308.15 | 0.65869 | 0.00184 | 453.15 | 0.51260 | 0.03037 |
| 313.15 | 0.65721 | 0.00210 | 458.15 | 0.50378 | 0.03267 |
| 318.15 | 0.65543 | 0.00239 | 463.15 | 0.49463 | 0.03514 |
| 323.15 | 0.65335 | 0.00271 | 468.15 | 0.48514 | 0.03777 |
| 328.15 | 0.65100 | 0.00307 | 473.15 | 0.47526 | 0.04059 |
| 333.15 | 0.64837 | 0.00345 | 478.15 | 0.46498 | 0.04360 |
| 338.15 | 0.64547 | 0.00388 | 483.15 | 0.45426 | 0.04683 |
| 343.15 | 0.64231 | 0.00434 | 488.15 | 0.44303 | 0.05031 |
| 348.15 | 0.63889 | 0.00485 | 493.15 | 0.43125 | 0.05404 |
| 353.15 | 0.63523 | 0.00540 | 498.15 | 0.41884 | 0.05828 |
| 358.15 | 0.63132 | 0.00599 | 503.15 | 0.40567 | 0.06267 |
| 363.15 | 0.62718 | 0.00664 | 508.15 | 0.39158 | 0.06743 |
| 368.15 | 0.62279 | 0.00733 | 513.15 | 0.37634 | 0.07261 |
| 373.15 | 0.61818 | 0.00808 | 518.15 | 0.36008 | 0.07810 |
| 378.15 | 0.61334 | 0.00888 | 523.15 | 0.34117 | 0.08432 |
| 383.15 | 0.60826 | 0.00975 | 528.15 | 0.31488 | 0.09167 |
| 388.15 | 0.60297 | 0.01067 | 533.15 | 0.27421 | 0.10002 |
| 393.15 | 0.59744 | 0.01167 | | | |
| toluene | | | | | |
| 253.15 | 0.77877 | 0.00012 | 433.15 | 0.72548 | 0.01332 |
| 258.15 | 0.78205 | 0.00015 | 438.15 | 0.72045 | 0.01440 |
| 263.15 | 0.78490 | 0.00019 | 443.15 | 0.71524 | 0.01553 |
| 268.15 | 0.78735 | 0.00023 | 448.15 | 0.70986 | 0.01675 |
| 273.15 | 0.78942 | 0.00028 | 453.15 | 0.70429 | 0.01803 |
| 278.15 | 0.79113 | 0.00034 | 458.15 | 0.69855 | 0.01938 |
| 283.15 | 0.79250 | 0.00040 | 463.15 | 0.69261 | 0.02081 |
| 288.15 | 0.79354 | 0.00048 | 468.15 | 0.68648 | 0.02232 |
| 293.15 | 0.79426 | 0.00057 | 473.15 | 0.68015 | 0.02392 |
| 298.15 | 0.79470 | 0.00067 | 478.15 | 0.67361 | 0.02561 |
| 303.15 | 0.79485 | 0.00078 | 483.15 | 0.66686 | 0.02740 |
| 308.15 | 0.79473 | 0.00091 | 488.15 | 0.65988 | 0.02929 |
| 313.15 | 0.79435 | 0.00105 | 493.15 | 0.65268 | 0.03128 |
| 318.15 | 0.79372 | 0.00121 | 498.15 | 0.64524 | 0.03339 |
| 323.15 | 0.79286 | 0.00139 | 503.15 | 0.63754 | 0.03563 |
| 328.15 | 0.79176 | 0.00159 | 508.15 | 0.62958 | 0.03799 |
| 333.15 | 0.79045 | 0.00182 | 513.15 | 0.62135 | 0.04047 |
| 338.15 | 0.78893 | 0.00206 | 518.15 | 0.61273 | 0.04311 |
| 343.15 | 0.78719 | 0.00233 | 523.15 | 0.60394 | 0.04591 |
| 348.15 | 0.78527 | 0.00263 | 528.15 | 0.59474 | 0.04888 |
| 353.15 | 0.78315 | 0.00295 | 533.15 | 0.58520 | 0.05203 |

| | | | | | |
|---------------|---------|---------|--------|---------|---------|
| 358.15 | 0.78083 | 0.00330 | 538.15 | 0.57532 | 0.05538 |
| 363.15 | 0.77834 | 0.00369 | 543.15 | 0.56503 | 0.05893 |
| 368.15 | 0.77566 | 0.00410 | 548.15 | 0.55429 | 0.06271 |
| 373.15 | 0.77281 | 0.00455 | 553.15 | 0.54307 | 0.06675 |
| 378.15 | 0.76978 | 0.00504 | 558.15 | 0.53142 | 0.07105 |
| 383.15 | 0.76658 | 0.00557 | 563.15 | 0.51906 | 0.07566 |
| 388.15 | 0.76322 | 0.00613 | 568.15 | 0.50600 | 0.08060 |
| 393.15 | 0.75969 | 0.00673 | 573.15 | 0.49213 | 0.08591 |
| 398.15 | 0.75599 | 0.00738 | 578.15 | 0.47770 | 0.09146 |
| 403.15 | 0.75213 | 0.00808 | 583.15 | 0.46168 | 0.09748 |
| 408.15 | 0.74810 | 0.00882 | 588.15 | 0.44405 | 0.10412 |
| 413.15 | 0.74391 | 0.00961 | 593.15 | 0.42416 | 0.11123 |
| 418.15 | 0.73955 | 0.01045 | 598.15 | 0.40041 | 0.11916 |
| 423.15 | 0.73503 | 0.01135 | 603.15 | 0.36870 | 0.12821 |
| 428.15 | 0.73034 | 0.01231 | | | |
| ethylbenzene | | | | | |
| 253.15 | 0.84850 | 0.00007 | 458.15 | 0.80472 | 0.01460 |
| 258.15 | 0.85165 | 0.00009 | 463.15 | 0.80064 | 0.01566 |
| 263.15 | 0.85450 | 0.00011 | 468.15 | 0.79643 | 0.01681 |
| 268.15 | 0.85699 | 0.00014 | 473.15 | 0.79208 | 0.01802 |
| 273.15 | 0.85915 | 0.00017 | 478.15 | 0.78758 | 0.01930 |
| 278.15 | 0.86099 | 0.00021 | 483.15 | 0.78294 | 0.02065 |
| 283.15 | 0.86254 | 0.00025 | 488.15 | 0.77814 | 0.02207 |
| 288.15 | 0.86382 | 0.00030 | 493.15 | 0.77319 | 0.02356 |
| 293.15 | 0.86483 | 0.00036 | 498.15 | 0.76808 | 0.02513 |
| 298.15 | 0.86560 | 0.00043 | 503.15 | 0.76280 | 0.02678 |
| 303.15 | 0.86613 | 0.00051 | 508.15 | 0.75735 | 0.02851 |
| 308.15 | 0.86645 | 0.00060 | 513.15 | 0.75172 | 0.03034 |
| 313.15 | 0.86655 | 0.00070 | 518.15 | 0.74591 | 0.03226 |
| 318.15 | 0.86646 | 0.00082 | 523.15 | 0.73991 | 0.03427 |
| 323.15 | 0.86619 | 0.00094 | 528.15 | 0.73371 | 0.03639 |
| 328.15 | 0.86573 | 0.00109 | 533.15 | 0.72731 | 0.03863 |
| 333.15 | 0.86510 | 0.00125 | 538.15 | 0.72068 | 0.04097 |
| 338.15 | 0.86430 | 0.00143 | 543.15 | 0.71384 | 0.04344 |
| 343.15 | 0.86334 | 0.00162 | 548.15 | 0.70677 | 0.04604 |
| 348.15 | 0.86224 | 0.00184 | 553.15 | 0.69945 | 0.04877 |
| 353.15 | 0.86098 | 0.00208 | 558.15 | 0.69187 | 0.05164 |
| 358.15 | 0.85958 | 0.00234 | 563.15 | 0.68402 | 0.05467 |
| 363.15 | 0.85804 | 0.00263 | 568.15 | 0.67588 | 0.05786 |
| 368.15 | 0.85636 | 0.00294 | 573.15 | 0.66744 | 0.06122 |
| 373.15 | 0.85456 | 0.00328 | 578.15 | 0.65868 | 0.06477 |
| 378.15 | 0.85262 | 0.00365 | 583.15 | 0.64957 | 0.06852 |
| 383.15 | 0.85055 | 0.00404 | 588.15 | 0.64007 | 0.07248 |
| 388.15 | 0.84836 | 0.00447 | 593.15 | 0.63019 | 0.07668 |
| 393.15 | 0.84604 | 0.00493 | 598.15 | 0.61987 | 0.08114 |
| 398.15 | 0.84360 | 0.00542 | 603.15 | 0.60907 | 0.08591 |
| 403.15 | 0.84104 | 0.00595 | 608.15 | 0.59803 | 0.09046 |
| 408.15 | 0.83835 | 0.00652 | 613.15 | 0.58588 | 0.09590 |
| 413.15 | 0.83555 | 0.00713 | 618.15 | 0.57329 | 0.10177 |
| 418.15 | 0.83262 | 0.00777 | 623.15 | 0.56001 | 0.10831 |
| 423.15 | 0.82957 | 0.00846 | 628.15 | 0.54616 | 0.11476 |
| 428.15 | 0.82640 | 0.00919 | 633.15 | 0.53088 | 0.12181 |
| 433.15 | 0.82310 | 0.00997 | 638.15 | 0.51456 | 0.12942 |
| 438.15 | 0.81968 | 0.01079 | 643.15 | 0.49620 | 0.13785 |
| 443.15 | 0.81613 | 0.01167 | 648.15 | 0.47535 | 0.14688 |
| 448.15 | 0.81246 | 0.01259 | 653.15 | 0.45022 | 0.15685 |
| 453.15 | 0.80865 | 0.01357 | 658.15 | 0.41490 | 0.16806 |
| propylbenzene | | | | | |
| 253.15 | 0.89840 | 0.00005 | 483.15 | 0.86181 | 0.01673 |
| 258.15 | 0.90127 | 0.00006 | 488.15 | 0.85857 | 0.01789 |

| | | | | | |
|--------|---------|------------------|--------|---------|---------|
| 263.15 | 0.90382 | 0.00007 | 493.15 | 0.85521 | 0.01910 |
| 268.15 | 0.90606 | 0.00009 | 498.15 | 0.85174 | 0.02038 |
| 273.15 | 0.90802 | 0.00011 | 503.15 | 0.84816 | 0.02172 |
| 278.15 | 0.90972 | 0.00014 | 508.15 | 0.84446 | 0.02313 |
| 283.15 | 0.91117 | 0.00017 | 513.15 | 0.84064 | 0.02460 |
| 288.15 | 0.91240 | 0.00021 | 518.15 | 0.83669 | 0.02614 |
| 293.15 | 0.91342 | 0.00025 | 523.15 | 0.83261 | 0.02776 |
| 298.15 | 0.91424 | 0.00030 | 528.15 | 0.82841 | 0.02946 |
| 303.15 | 0.91487 | 0.00036 | 533.15 | 0.82406 | 0.03123 |
| 308.15 | 0.91534 | 0.00043 | 538.15 | 0.81957 | 0.03309 |
| 313.15 | 0.91564 | 0.00050 | 543.15 | 0.81493 | 0.03503 |
| 318.15 | 0.91579 | 0.00059 | 548.15 | 0.81014 | 0.03707 |
| 323.15 | 0.91580 | 0.00069 | 553.15 | 0.80519 | 0.03920 |
| 328.15 | 0.91567 | 0.00080 | 558.15 | 0.80008 | 0.04143 |
| 333.15 | 0.91541 | 0.00092 | 563.15 | 0.79479 | 0.04376 |
| 338.15 | 0.91503 | 0.00106 | 568.15 | 0.78933 | 0.04621 |
| 343.15 | 0.91453 | 0.00121 | 573.15 | 0.78369 | 0.04876 |
| 348.15 | 0.91391 | 0.00138 | 578.15 | 0.77785 | 0.05144 |
| 353.15 | 0.91319 | 0.00157 | 583.15 | 0.77180 | 0.05424 |
| 358.15 | 0.91236 | 0.00178 | 588.15 | 0.76555 | 0.05717 |
| 363.15 | 0.91143 | 0.00200 | 593.15 | 0.75905 | 0.06007 |
| 368.15 | 0.91040 | 0.00225 | 598.15 | 0.75234 | 0.06327 |
| 373.15 | 0.90928 | 0.00252 | 603.15 | 0.74538 | 0.06663 |
| 378.15 | 0.90806 | 0.00281 | 608.15 | 0.73817 | 0.07015 |
| 383.15 | 0.90675 | 0.00313 | 613.15 | 0.73067 | 0.07385 |
| 388.15 | 0.90535 | 0.00348 | 618.15 | 0.72289 | 0.07773 |
| 393.15 | 0.90386 | 0.00385 | 623.15 | 0.71474 | 0.08180 |
| 398.15 | 0.90229 | 0.00425 | 628.15 | 0.70631 | 0.08607 |
| 403.15 | 0.90062 | 0.00468 | 633.15 | 0.69751 | 0.09058 |
| 408.15 | 0.89887 | 0.00514 | 638.15 | 0.68833 | 0.09532 |
| 413.15 | 0.89703 | 0.00563 | 643.15 | 0.67873 | 0.10032 |
| 418.15 | 0.89510 | 0.00616 | 648.15 | 0.66867 | 0.10559 |
| 423.15 | 0.89309 | 0.00672 | 653.15 | 0.65809 | 0.11116 |
| 428.15 | 0.89099 | 0.00732 | 658.15 | 0.64725 | 0.11689 |
| 433.15 | 0.88880 | 0.00796 | 663.15 | 0.63549 | 0.12311 |
| 438.15 | 0.88653 | 0.00863 | 668.15 | 0.62300 | 0.12982 |
| 443.15 | 0.88416 | 0.00935 | 673.15 | 0.60966 | 0.13687 |
| 448.15 | 0.88170 | 0.01011 | 678.15 | 0.59535 | 0.14440 |
| 453.15 | 0.87915 | 0.01091 | 683.15 | 0.57973 | 0.15245 |
| 458.15 | 0.87651 | 0.01175 | 688.15 | 0.56250 | 0.16109 |
| 463.15 | 0.87377 | 0.01265 | 693.15 | 0.54303 | 0.17040 |
| 468.15 | 0.87093 | 0.01359 | 698.15 | 0.52006 | 0.18061 |
| 473.15 | 0.86800 | 0.01459 | 703.15 | 0.49034 | 0.19174 |
| 478.15 | 0.86495 | 0.01563 | | | |
| | | <i>p</i> -xylene | | | |
| 253.15 | 0.86400 | 0.00006 | 463.15 | 0.81859 | 0.01412 |
| 258.15 | 0.86703 | 0.00007 | 468.15 | 0.81462 | 0.01518 |
| 263.15 | 0.86975 | 0.00009 | 473.15 | 0.81051 | 0.01629 |
| 268.15 | 0.87212 | 0.00011 | 478.15 | 0.80627 | 0.01746 |
| 273.15 | 0.87417 | 0.00014 | 483.15 | 0.80189 | 0.01870 |
| 278.15 | 0.87591 | 0.00017 | 488.15 | 0.79737 | 0.02000 |
| 283.15 | 0.87736 | 0.00021 | 493.15 | 0.79270 | 0.02137 |
| 288.15 | 0.87855 | 0.00025 | 498.15 | 0.78788 | 0.02281 |
| 293.15 | 0.87950 | 0.00030 | 503.15 | 0.78291 | 0.02433 |
| 298.15 | 0.88020 | 0.00036 | 508.15 | 0.77778 | 0.02593 |
| 303.15 | 0.88069 | 0.00042 | 513.15 | 0.77248 | 0.02760 |
| 308.15 | 0.88097 | 0.00050 | 518.15 | 0.76702 | 0.02936 |
| 313.15 | 0.88105 | 0.00059 | 523.15 | 0.76138 | 0.03122 |
| 318.15 | 0.88095 | 0.00069 | 528.15 | 0.75555 | 0.03316 |
| 323.15 | 0.88067 | 0.00080 | 533.15 | 0.74953 | 0.03521 |

| | | | | | |
|--------|---------|---------|--------|---------|---------|
| 328.15 | 0.88021 | 0.00092 | 538.15 | 0.74333 | 0.03741 |
| 333.15 | 0.87960 | 0.00107 | 543.15 | 0.73691 | 0.03967 |
| 338.15 | 0.87883 | 0.00122 | 548.15 | 0.73028 | 0.04204 |
| 343.15 | 0.87791 | 0.00140 | 553.15 | 0.72343 | 0.04453 |
| 348.15 | 0.87685 | 0.00159 | 558.15 | 0.71635 | 0.04716 |
| 353.15 | 0.87566 | 0.00180 | 563.15 | 0.70902 | 0.04991 |
| 358.15 | 0.87432 | 0.00203 | 568.15 | 0.70144 | 0.05282 |
| 363.15 | 0.87286 | 0.00229 | 573.15 | 0.69359 | 0.05587 |
| 368.15 | 0.87127 | 0.00257 | 578.15 | 0.68545 | 0.05910 |
| 373.15 | 0.86955 | 0.00287 | 583.15 | 0.67700 | 0.06250 |
| 378.15 | 0.86771 | 0.00320 | 588.15 | 0.66825 | 0.06612 |
| 383.15 | 0.86575 | 0.00356 | 593.15 | 0.65915 | 0.06991 |
| 388.15 | 0.86368 | 0.00394 | 598.15 | 0.64973 | 0.07400 |
| 393.15 | 0.86149 | 0.00436 | 603.15 | 0.63986 | 0.07824 |
| 398.15 | 0.85918 | 0.00481 | 608.15 | 0.62954 | 0.08274 |
| 403.15 | 0.85675 | 0.00529 | 613.15 | 0.61878 | 0.08750 |
| 408.15 | 0.85422 | 0.00580 | 618.15 | 0.60746 | 0.09258 |
| 413.15 | 0.85157 | 0.00635 | 623.15 | 0.59558 | 0.09803 |
| 418.15 | 0.84880 | 0.00694 | 628.15 | 0.58303 | 0.10379 |
| 423.15 | 0.84592 | 0.00753 | 633.15 | 0.57008 | 0.10976 |
| 428.15 | 0.84292 | 0.00819 | 638.15 | 0.55592 | 0.11627 |
| 433.15 | 0.83981 | 0.00890 | 643.15 | 0.54068 | 0.12325 |
| 438.15 | 0.83658 | 0.00965 | 648.15 | 0.52410 | 0.13086 |
| 443.15 | 0.83323 | 0.01045 | 653.15 | 0.50576 | 0.13902 |
| 448.15 | 0.82977 | 0.01129 | 658.15 | 0.48495 | 0.14797 |
| 453.15 | 0.82618 | 0.01218 | 663.15 | 0.46029 | 0.15754 |
| 458.15 | 0.82244 | 0.01313 | 668.15 | 0.42706 | 0.16845 |

TABLE 2S: Liquid–Liquid Phase Equilibria Predicted by the COSMO-RS for $\{x_1$ [bmim][CH₃SO₄] + (1- x_1) Hydrocarbon} Mixtures

| T (K) | x_1' | x_1'' | T (K) | x_1' | x_1'' |
|-------------------|---------|---------|---------|---------|---------|
| <i>n</i> -pentane | | | | | |
| 273.15 | 0.91543 | 0.00001 | 458.15 | 0.76408 | 0.00665 |
| 278.15 | 0.91385 | 0.00002 | 463.15 | 0.75707 | 0.00729 |
| 283.15 | 0.91214 | 0.00003 | 468.15 | 0.74987 | 0.00797 |
| 288.15 | 0.91028 | 0.00003 | 473.15 | 0.74249 | 0.00870 |
| 293.15 | 0.90830 | 0.00004 | 478.15 | 0.73493 | 0.00948 |
| 298.15 | 0.90618 | 0.00006 | 483.15 | 0.72718 | 0.01032 |
| 303.15 | 0.90393 | 0.00007 | 488.15 | 0.71923 | 0.01121 |
| 308.15 | 0.90154 | 0.00009 | 493.15 | 0.71109 | 0.01217 |
| 313.15 | 0.89902 | 0.00011 | 498.15 | 0.70274 | 0.01319 |
| 318.15 | 0.89637 | 0.00014 | 503.15 | 0.69419 | 0.01428 |
| 323.15 | 0.89358 | 0.00017 | 508.15 | 0.68543 | 0.01544 |
| 328.15 | 0.89066 | 0.00021 | 513.15 | 0.67644 | 0.01668 |
| 333.15 | 0.88760 | 0.00025 | 518.15 | 0.66724 | 0.01799 |
| 338.15 | 0.88441 | 0.00030 | 523.15 | 0.65780 | 0.01940 |
| 343.15 | 0.88108 | 0.00036 | 528.15 | 0.64812 | 0.02089 |
| 348.15 | 0.87762 | 0.00043 | 533.15 | 0.63820 | 0.02249 |
| 353.15 | 0.87401 | 0.00051 | 538.15 | 0.62802 | 0.02419 |
| 358.15 | 0.87027 | 0.00060 | 543.15 | 0.61758 | 0.02600 |
| 363.15 | 0.86639 | 0.00070 | 548.15 | 0.60686 | 0.02793 |
| 368.15 | 0.86236 | 0.00082 | 553.15 | 0.59585 | 0.02999 |
| 373.15 | 0.85819 | 0.00095 | 558.15 | 0.58452 | 0.03219 |
| 378.15 | 0.85388 | 0.00109 | 563.15 | 0.57288 | 0.03457 |
| 383.15 | 0.84943 | 0.00125 | 568.15 | 0.56073 | 0.03709 |
| 388.15 | 0.84482 | 0.00143 | 573.15 | 0.54837 | 0.03978 |
| 393.15 | 0.84007 | 0.00163 | 578.15 | 0.53561 | 0.04267 |
| 398.15 | 0.83517 | 0.00185 | 583.15 | 0.52239 | 0.04577 |
| 403.15 | 0.83012 | 0.00209 | 588.15 | 0.50873 | 0.04909 |
| 408.15 | 0.82492 | 0.00236 | 593.15 | 0.49451 | 0.05268 |
| 413.15 | 0.81956 | 0.00265 | 598.15 | 0.47973 | 0.05660 |
| 418.15 | 0.81404 | 0.00296 | 603.15 | 0.46428 | 0.06080 |
| 423.15 | 0.80837 | 0.00331 | 608.15 | 0.44796 | 0.06536 |
| 428.15 | 0.80254 | 0.00368 | 613.15 | 0.43072 | 0.07031 |
| 433.15 | 0.79655 | 0.00409 | 618.15 | 0.41219 | 0.07575 |
| 438.15 | 0.79039 | 0.00452 | 623.15 | 0.39198 | 0.08172 |
| 443.15 | 0.78407 | 0.00500 | 628.15 | 0.36936 | 0.08832 |
| 448.15 | 0.77758 | 0.00551 | 633.15 | 0.34234 | 0.09573 |
| 453.15 | 0.77092 | 0.00606 | 638.15 | 0.30216 | 0.10441 |
| cyclohexane | | | | | |
| 268.15 | 0.91443 | 0.00001 | 458.15 | 0.75675 | 0.00592 |
| 273.15 | 0.91285 | 0.00001 | 463.15 | 0.74965 | 0.00649 |
| 278.15 | 0.91114 | 0.00001 | 468.15 | 0.74237 | 0.00711 |
| 283.15 | 0.90929 | 0.00002 | 473.15 | 0.73491 | 0.00777 |
| 288.15 | 0.90730 | 0.00003 | 478.15 | 0.72728 | 0.00846 |
| 293.15 | 0.90518 | 0.00003 | 483.15 | 0.71946 | 0.00922 |
| 298.15 | 0.90292 | 0.00004 | 488.15 | 0.71146 | 0.01003 |
| 303.15 | 0.90053 | 0.00006 | 493.15 | 0.70328 | 0.01090 |
| 308.15 | 0.89801 | 0.00007 | 498.15 | 0.69489 | 0.01182 |
| 313.15 | 0.89535 | 0.00009 | 503.15 | 0.68632 | 0.01281 |
| 318.15 | 0.89257 | 0.00011 | 508.15 | 0.67754 | 0.01387 |
| 323.15 | 0.88964 | 0.00014 | 513.15 | 0.66858 | 0.01499 |
| 328.15 | 0.88659 | 0.00017 | 518.15 | 0.65939 | 0.01619 |
| 333.15 | 0.88340 | 0.00021 | 523.15 | 0.64998 | 0.01747 |
| 338.15 | 0.88007 | 0.00025 | 528.15 | 0.64034 | 0.01883 |
| 343.15 | 0.87660 | 0.00030 | 533.15 | 0.63048 | 0.02032 |
| 348.15 | 0.87300 | 0.00036 | 538.15 | 0.62038 | 0.02188 |
| 353.15 | 0.86926 | 0.00043 | 543.15 | 0.61003 | 0.02353 |

| | | | | | |
|--------------|---------|---------|--------|---------|---------|
| 358.15 | 0.86539 | 0.00051 | 548.15 | 0.59940 | 0.02530 |
| 363.15 | 0.86137 | 0.00060 | 553.15 | 0.58854 | 0.02724 |
| 368.15 | 0.85721 | 0.00070 | 558.15 | 0.57739 | 0.02926 |
| 373.15 | 0.85291 | 0.00081 | 563.15 | 0.56596 | 0.03142 |
| 378.15 | 0.84846 | 0.00094 | 568.15 | 0.55402 | 0.03371 |
| 383.15 | 0.84387 | 0.00108 | 573.15 | 0.54194 | 0.03621 |
| 388.15 | 0.83914 | 0.00124 | 578.15 | 0.52950 | 0.03886 |
| 393.15 | 0.83425 | 0.00141 | 583.15 | 0.51669 | 0.04170 |
| 398.15 | 0.82922 | 0.00161 | 588.15 | 0.50348 | 0.04476 |
| 403.15 | 0.82405 | 0.00182 | 593.15 | 0.49011 | 0.04803 |
| 408.15 | 0.81872 | 0.00206 | 598.15 | 0.47597 | 0.05159 |
| 413.15 | 0.81323 | 0.00232 | 603.15 | 0.46127 | 0.05544 |
| 418.15 | 0.80760 | 0.00260 | 608.15 | 0.44592 | 0.05962 |
| 423.15 | 0.80180 | 0.00291 | 613.15 | 0.42981 | 0.06418 |
| 428.15 | 0.79585 | 0.00324 | 618.15 | 0.41279 | 0.06916 |
| 433.15 | 0.78974 | 0.00361 | 623.15 | 0.39407 | 0.07465 |
| 438.15 | 0.78348 | 0.00400 | 628.15 | 0.37425 | 0.08071 |
| 443.15 | 0.77704 | 0.00443 | 633.15 | 0.35272 | 0.08743 |
| 448.15 | 0.77044 | 0.00489 | 638.15 | 0.32670 | 0.09504 |
| 453.15 | 0.76368 | 0.00539 | 643.15 | 0.28960 | 0.10385 |
| cycloheptane | | | | | |
| 268.15 | 0.94508 | 0.00001 | 468.15 | 0.81152 | 0.00698 |
| 273.15 | 0.94394 | 0.00001 | 473.15 | 0.80544 | 0.00763 |
| 278.15 | 0.94269 | 0.00001 | 478.15 | 0.79919 | 0.00832 |
| 283.15 | 0.94135 | 0.00002 | 483.15 | 0.79277 | 0.00905 |
| 288.15 | 0.93990 | 0.00003 | 488.15 | 0.78617 | 0.00984 |
| 293.15 | 0.93835 | 0.00003 | 493.15 | 0.77940 | 0.01068 |
| 298.15 | 0.93670 | 0.00004 | 498.15 | 0.77245 | 0.01157 |
| 303.15 | 0.93494 | 0.00006 | 503.15 | 0.76531 | 0.01252 |
| 308.15 | 0.93300 | 0.00008 | 508.15 | 0.75799 | 0.01353 |
| 313.15 | 0.93113 | 0.00009 | 513.15 | 0.75047 | 0.01461 |
| 318.15 | 0.92906 | 0.00011 | 518.15 | 0.74275 | 0.01576 |
| 323.15 | 0.92689 | 0.00014 | 523.15 | 0.73483 | 0.01697 |
| 328.15 | 0.92461 | 0.00017 | 528.15 | 0.72670 | 0.01827 |
| 333.15 | 0.92223 | 0.00021 | 533.15 | 0.71835 | 0.01964 |
| 338.15 | 0.91974 | 0.00025 | 538.15 | 0.70978 | 0.02110 |
| 343.15 | 0.91713 | 0.00030 | 543.15 | 0.70098 | 0.02264 |
| 348.15 | 0.91442 | 0.00036 | 548.15 | 0.69195 | 0.02429 |
| 353.15 | 0.91159 | 0.00043 | 553.15 | 0.68267 | 0.02603 |
| 358.15 | 0.90865 | 0.00050 | 558.15 | 0.67313 | 0.02789 |
| 363.15 | 0.90559 | 0.00059 | 563.15 | 0.66334 | 0.02986 |
| 368.15 | 0.90242 | 0.00069 | 568.15 | 0.65327 | 0.03195 |
| 373.15 | 0.89912 | 0.00080 | 573.15 | 0.64291 | 0.03417 |
| 378.15 | 0.89571 | 0.00093 | 578.15 | 0.63225 | 0.03653 |
| 383.15 | 0.89217 | 0.00107 | 583.15 | 0.62128 | 0.03904 |
| 388.15 | 0.88851 | 0.00122 | 588.15 | 0.60996 | 0.04172 |
| 393.15 | 0.88473 | 0.00140 | 593.15 | 0.59830 | 0.04458 |
| 398.15 | 0.88082 | 0.00159 | 598.15 | 0.58626 | 0.04763 |
| 403.15 | 0.87677 | 0.00180 | 603.15 | 0.57381 | 0.05089 |
| 408.15 | 0.87260 | 0.00203 | 608.15 | 0.56090 | 0.05438 |
| 413.15 | 0.86830 | 0.00228 | 613.15 | 0.54753 | 0.05811 |
| 418.15 | 0.86386 | 0.00256 | 618.15 | 0.53362 | 0.06215 |
| 423.15 | 0.85928 | 0.00287 | 623.15 | 0.51911 | 0.06647 |
| 428.15 | 0.85456 | 0.00320 | 628.15 | 0.50391 | 0.07115 |
| 433.15 | 0.84970 | 0.00355 | 633.15 | 0.48792 | 0.07621 |
| 438.15 | 0.84470 | 0.00394 | 638.15 | 0.47099 | 0.08170 |
| 443.15 | 0.83955 | 0.00436 | 643.15 | 0.45290 | 0.08769 |
| 448.15 | 0.83425 | 0.00481 | 648.15 | 0.43330 | 0.09426 |
| 453.15 | 0.82881 | 0.00530 | 653.15 | 0.41101 | 0.10150 |
| 458.15 | 0.82320 | 0.00582 | 658.15 | 0.38578 | 0.10956 |

| | | | | | |
|--------|---------|---------|---------------|---------|---------|
| 463.15 | 0.81744 | 0.00638 | 663.15 | 0.35312 | 0.11868 |
| | | | benzene | | |
| 253.15 | 0.47406 | 0.00217 | 318.15 | 0.38087 | 0.01404 |
| 258.15 | 0.46970 | 0.00257 | 323.15 | 0.37035 | 0.01587 |
| 263.15 | 0.46488 | 0.00303 | 328.15 | 0.35928 | 0.01790 |
| 268.15 | 0.45958 | 0.00355 | 333.15 | 0.34762 | 0.02017 |
| 273.15 | 0.45380 | 0.00415 | 338.15 | 0.33533 | 0.02270 |
| 278.15 | 0.44755 | 0.00482 | 343.15 | 0.32229 | 0.02552 |
| 283.15 | 0.44084 | 0.00557 | 348.15 | 0.30840 | 0.02868 |
| 288.15 | 0.43367 | 0.00642 | 353.15 | 0.29345 | 0.03223 |
| 293.15 | 0.42605 | 0.00737 | 358.15 | 0.27715 | 0.03628 |
| 298.15 | 0.41796 | 0.00843 | 363.15 | 0.25888 | 0.04084 |
| 303.15 | 0.40962 | 0.00959 | 368.15 | 0.23748 | 0.04607 |
| 308.15 | 0.40038 | 0.01092 | 373.15 | 0.20776 | 0.05228 |
| 313.15 | 0.39087 | 0.01240 | | | |
| | | | toluene | | |
| 253.15 | 0.64925 | 0.00090 | 348.15 | 0.53797 | 0.01323 |
| 258.15 | 0.64704 | 0.00108 | 353.15 | 0.52823 | 0.01474 |
| 263.15 | 0.64449 | 0.00129 | 358.15 | 0.51810 | 0.01640 |
| 268.15 | 0.64148 | 0.00154 | 363.15 | 0.50755 | 0.01816 |
| 273.15 | 0.63802 | 0.00181 | 368.15 | 0.49659 | 0.02012 |
| 278.15 | 0.63412 | 0.00213 | 373.15 | 0.48518 | 0.02227 |
| 283.15 | 0.62980 | 0.00249 | 378.15 | 0.47330 | 0.02460 |
| 288.15 | 0.62506 | 0.00290 | 383.15 | 0.46091 | 0.02715 |
| 293.15 | 0.61991 | 0.00335 | 388.15 | 0.44798 | 0.02993 |
| 298.15 | 0.61436 | 0.00386 | 393.15 | 0.43445 | 0.03297 |
| 303.15 | 0.60843 | 0.00444 | 398.15 | 0.42021 | 0.03628 |
| 308.15 | 0.60210 | 0.00507 | 403.15 | 0.40524 | 0.03991 |
| 313.15 | 0.59539 | 0.00578 | 408.15 | 0.38933 | 0.04391 |
| 318.15 | 0.58831 | 0.00656 | 413.15 | 0.37228 | 0.04831 |
| 323.15 | 0.58090 | 0.00743 | 418.15 | 0.35369 | 0.05314 |
| 328.15 | 0.57307 | 0.00838 | 423.15 | 0.33379 | 0.05840 |
| 333.15 | 0.56486 | 0.00942 | 428.15 | 0.30868 | 0.06470 |
| 338.15 | 0.55628 | 0.01058 | 433.15 | 0.27548 | 0.07163 |
| 343.15 | 0.54731 | 0.01184 | | | |
| | | | ethylbenzene | | |
| 253.15 | 0.75298 | 0.00055 | 368.15 | 0.64421 | 0.01375 |
| 258.15 | 0.75214 | 0.00067 | 373.15 | 0.63540 | 0.01520 |
| 263.15 | 0.75090 | 0.00081 | 378.15 | 0.62647 | 0.01671 |
| 268.15 | 0.74924 | 0.00097 | 383.15 | 0.61721 | 0.01839 |
| 273.15 | 0.74719 | 0.00116 | 388.15 | 0.60760 | 0.02022 |
| 278.15 | 0.74476 | 0.00137 | 393.15 | 0.59763 | 0.02220 |
| 283.15 | 0.74196 | 0.00161 | 398.15 | 0.58729 | 0.02432 |
| 288.15 | 0.73880 | 0.00189 | 403.15 | 0.57656 | 0.02665 |
| 293.15 | 0.73529 | 0.00220 | 408.15 | 0.56543 | 0.02911 |
| 298.15 | 0.73144 | 0.00255 | 413.15 | 0.55387 | 0.03179 |
| 303.15 | 0.72725 | 0.00294 | 418.15 | 0.54183 | 0.03455 |
| 308.15 | 0.72273 | 0.00338 | 423.15 | 0.52929 | 0.03764 |
| 313.15 | 0.71789 | 0.00387 | 428.15 | 0.51622 | 0.04103 |
| 318.15 | 0.71273 | 0.00441 | 433.15 | 0.50250 | 0.04466 |
| 323.15 | 0.70726 | 0.00501 | 438.15 | 0.48821 | 0.04860 |
| 328.15 | 0.70147 | 0.00568 | 443.15 | 0.47306 | 0.05288 |
| 333.15 | 0.69553 | 0.00638 | 448.15 | 0.45705 | 0.05753 |
| 338.15 | 0.68897 | 0.00718 | 453.15 | 0.43989 | 0.06261 |
| 343.15 | 0.68225 | 0.00806 | 458.15 | 0.42126 | 0.06821 |
| 348.15 | 0.67523 | 0.00904 | 463.15 | 0.40065 | 0.07431 |
| 353.15 | 0.66789 | 0.01009 | 468.15 | 0.37709 | 0.08090 |
| 358.15 | 0.66024 | 0.01122 | 473.15 | 0.34775 | 0.08848 |
| 363.15 | 0.65228 | 0.01245 | 478.15 | 0.29079 | 0.09787 |
| | | | propylbenzene | | |

| | | | | | |
|--------|---------|------------------|--------|---------|---------|
| 253.15 | 0.83191 | 0,00037 | 388.15 | 0.72909 | 0,01531 |
| 258.15 | 0.83180 | 0,00046 | 393.15 | 0.72168 | 0,01679 |
| 263.15 | 0.83133 | 0,00056 | 398.15 | 0.71400 | 0,01837 |
| 268.15 | 0.83052 | 0,00067 | 403.15 | 0.70604 | 0,02007 |
| 273.15 | 0.82938 | 0,00080 | 408.15 | 0.69779 | 0,02190 |
| 278.15 | 0.82793 | 0,00096 | 413.15 | 0.68925 | 0,02385 |
| 283.15 | 0.82618 | 0,00114 | 418.15 | 0.68040 | 0,02595 |
| 288.15 | 0.82413 | 0,00134 | 423.15 | 0.67121 | 0,02824 |
| 293.15 | 0.82181 | 0,00157 | 428.15 | 0.66170 | 0,03065 |
| 298.15 | 0.81921 | 0,00183 | 433.15 | 0.65184 | 0,03322 |
| 303.15 | 0.81634 | 0,00213 | 438.15 | 0.64161 | 0,03594 |
| 308.15 | 0.81321 | 0,00246 | 443.15 | 0.63099 | 0,03887 |
| 313.15 | 0.80982 | 0,00282 | 448.15 | 0.61995 | 0,04202 |
| 318.15 | 0.80617 | 0,00323 | 453.15 | 0.60846 | 0,04538 |
| 323.15 | 0.80228 | 0,00369 | 458.15 | 0.59650 | 0,04900 |
| 328.15 | 0.79813 | 0,00419 | 463.15 | 0.58399 | 0,05287 |
| 333.15 | 0.79374 | 0,00475 | 468.15 | 0.57092 | 0,05701 |
| 338.15 | 0.78910 | 0,00535 | 473.15 | 0.55717 | 0,06147 |
| 343.15 | 0.78421 | 0,00602 | 478.15 | 0.54269 | 0,06627 |
| 348.15 | 0.77908 | 0,00675 | 483.15 | 0.52732 | 0,07145 |
| 353.15 | 0.77371 | 0,00754 | 488.15 | 0.51088 | 0,07705 |
| 358.15 | 0.76809 | 0,00841 | 493.15 | 0.49336 | 0,08308 |
| 363.15 | 0.76222 | 0,00935 | 498.15 | 0.47414 | 0,08966 |
| 368.15 | 0.75610 | 0,01037 | 503.15 | 0.45308 | 0,09653 |
| 373.15 | 0.74973 | 0,01147 | 508.15 | 0.42707 | 0,10462 |
| 378.15 | 0.74311 | 0,01265 | 513.15 | 0.39603 | 0,11304 |
| 383.15 | 0.73623 | 0,01393 | | | |
| | | <i>p</i> -xylene | | | |
| 253.15 | 0.77803 | 0.00043 | 378.15 | 0.65889 | 0.0145 |
| 258.15 | 0.77730 | 0.00053 | 383.15 | 0.65018 | 0.01598 |
| 263.15 | 0.77616 | 0.00064 | 388.15 | 0.64114 | 0.01759 |
| 268.15 | 0.77463 | 0.00078 | 393.15 | 0.63178 | 0.01932 |
| 273.15 | 0.77272 | 0.00094 | 398.15 | 0.62213 | 0.02119 |
| 278.15 | 0.77045 | 0.00111 | 403.15 | 0.61209 | 0.0232 |
| 283.15 | 0.76782 | 0.00132 | 408.15 | 0.60169 | 0.02537 |
| 288.15 | 0.76485 | 0.00155 | 413.15 | 0.59095 | 0.02770 |
| 293.15 | 0.76154 | 0.00182 | 418.15 | 0.57979 | 0.03022 |
| 298.15 | 0.75791 | 0.00212 | 423.15 | 0.5682 | 0.03291 |
| 303.15 | 0.75395 | 0.00245 | 428.15 | 0.55617 | 0.03584 |
| 308.15 | 0.74969 | 0.00283 | 433.15 | 0.54367 | 0.03895 |
| 313.15 | 0.74512 | 0.00325 | 438.15 | 0.53067 | 0.04236 |
| 318.15 | 0.74025 | 0.00372 | 443.15 | 0.51706 | 0.04604 |
| 323.15 | 0.73508 | 0.00424 | 448.15 | 0.50291 | 0.04995 |
| 328.15 | 0.72962 | 0.00482 | 453.15 | 0.48793 | 0.05427 |
| 333.15 | 0.72387 | 0.00545 | 458.15 | 0.47214 | 0.05895 |
| 338.15 | 0.71783 | 0.00615 | 463.15 | 0.45532 | 0.06406 |
| 343.15 | 0.71151 | 0.00691 | 468.15 | 0.4372 | 0.06967 |
| 348.15 | 0.70487 | 0.00775 | 473.15 | 0.4174 | 0.07582 |
| 353.15 | 0.69795 | 0.00867 | 478.15 | 0.3952 | 0.08261 |
| 358.15 | 0.69075 | 0.00966 | 483.15 | 0.37 | 0.08996 |
| 363.15 | 0.68324 | 0.01075 | 488.15 | 0.3378 | 0.0984 |
| 368.15 | 0.67543 | 0.01192 | 493.15 | 0.3052 | 0.11024 |
| 373.15 | 0.66728 | 0.01313 | | | |

Captions to the Figures:

Fig. 1S Thermogravimetric analysis (TGA) curves of the thermal degradation of (—) [mmim][CH₃SO₄] and (---) [bmim][CH₃SO₄].

Fig. 2S Decomposition (d(mass loss)/dT) curves of the thermal degradation of 1,3-dialkylimidazole methylsulfates: (—) [mmim][CH₃SO₄] and (---) [bmim][CH₃SO₄].

Fig. 3S Liquid–liquid phase equilibria diagram of binary systems: $\{x_1$ [bmim][CH₃SO₄] + (1- x_1) *n*-alkane}: □, *n*-pentane; *, *n*-hexane; —, *n*-heptane; ○, *n*-octane; ■, *n*-decane; dotted line, boiling temperature of a solvent.

Fig. 4S Liquid–liquid phase equilibria diagram of binary systems: $\{x_1$ [mmim][CH₃SO₄] + (1- x_1) cycloalkanes}: Δ, cyclohexane; ○, cycloheptane; solid line, calculated by the COSMO-RS; dotted line, boiling temperature of a solvent.

Fig. 5S Liquid–liquid phase equilibria diagram of binary systems: $\{x_1$ [bmim][CH₃SO₄] + (1- x_1) cycloalkane}: ■, cyclohexane; ●, cycloheptane; solid line, calculated by the COSMO-RS; dotted line, boiling temperature of a solvent.

Fig. 6S Liquid–liquid phase equilibria diagrams: $\{x_1$ [mmim][CH₃SO₄] + (1- x_1) xylene}: —, *o*-xylene; *, *m*-xylene; x, *p*-xylene; dotted line, boiling temperature of a solvent.

Fig. 7S Solubility of x, [mmim][CH₃SO₄](1) or ■, [bmim][CH₃SO₄](1) in *n*-decane (2); lines are calculated by the COSMO-RS: (—) [mmim][CH₃SO₄] and (---) [bmim][CH₃SO₄]; dotted line, boiling temperature of *n*-decane.

Fig. 8S Solubility of, \diamond [mmim][CH₃SO₄] (1) or \blacklozenge , [bmim][CH₃SO₄] (1) in propylbenzene (2); lines are calculated by the COSMO-RS: (—) [mmim][CH₃SO₄] and (---) [bmim][CH₃SO₄]; dotted line, boiling temperature of propylbenzene.

Fig. 9S Solubility of, x [mmim][CH₃SO₄] (1) or *, [bmim][CH₃SO₄] (1) in *p*-xylene (2); lines are calculated by the COSMO-RS: (—) [mmim][CH₃SO₄] and (---) [bmim][CH₃SO₄]; dotted line, boiling temperature of *p*-xylene.

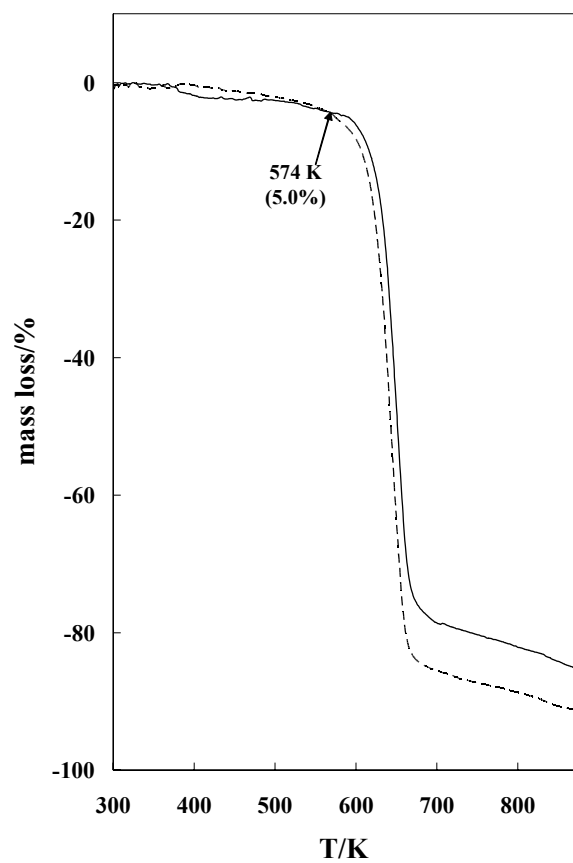


Figure 1S.

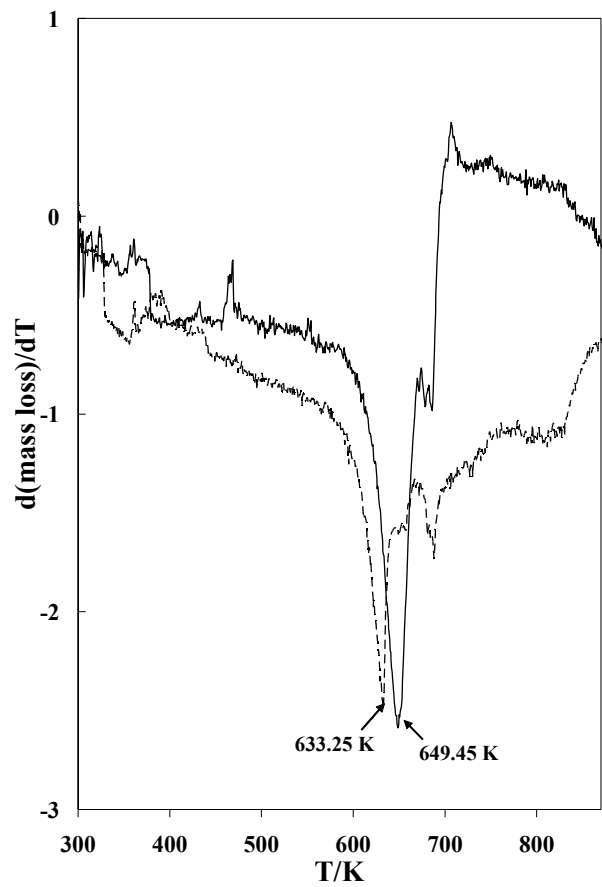


Figure 2S.

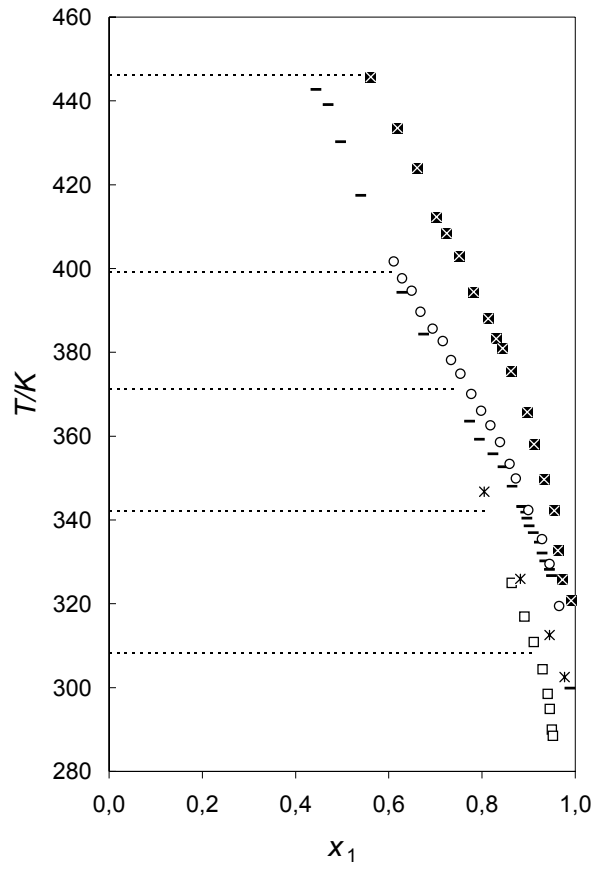


Figure 3S.

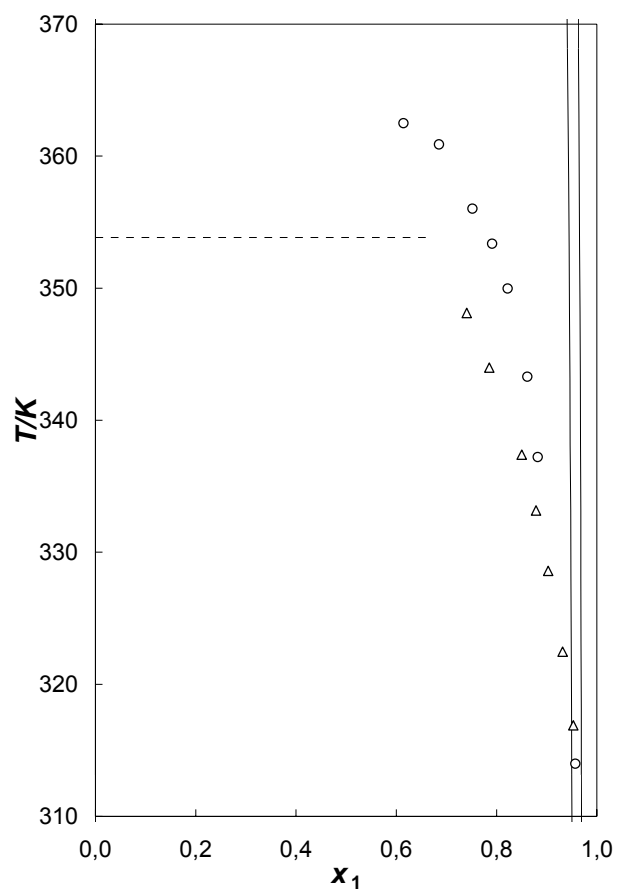


Figure 4S.

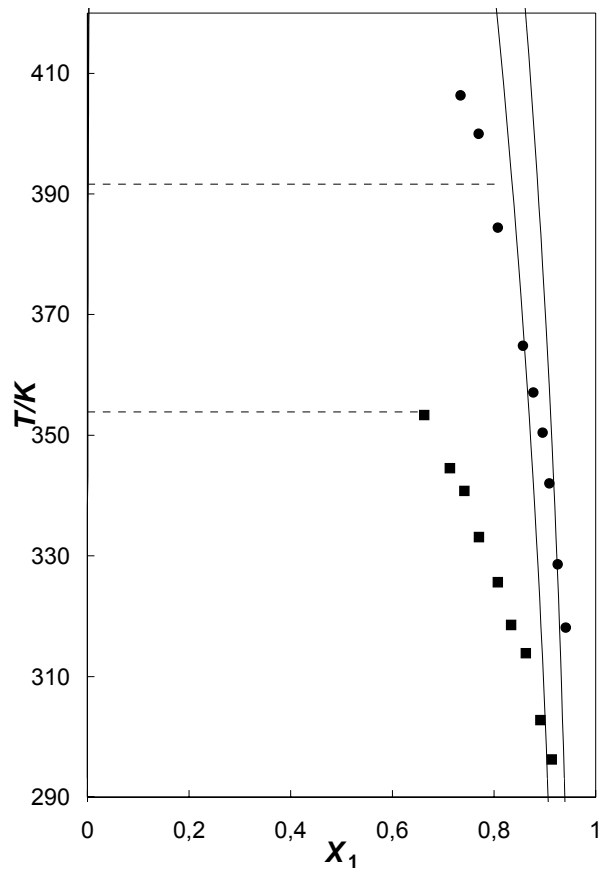


Figure 5S.

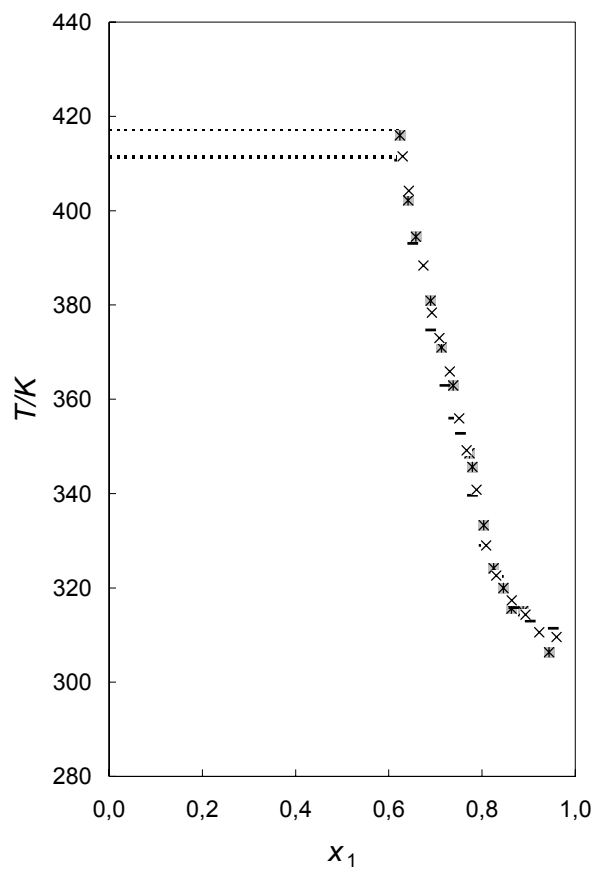


Figure 6S.

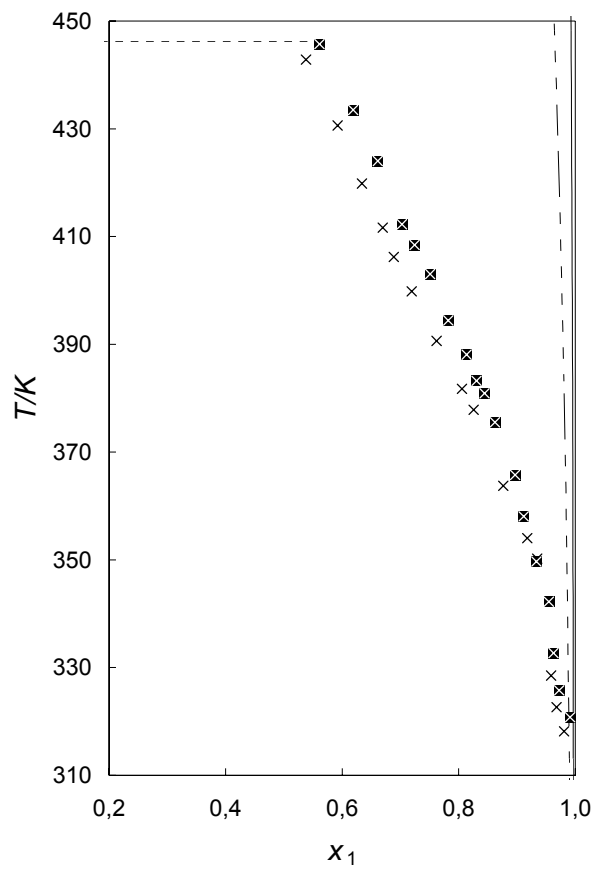


Figure 7S.

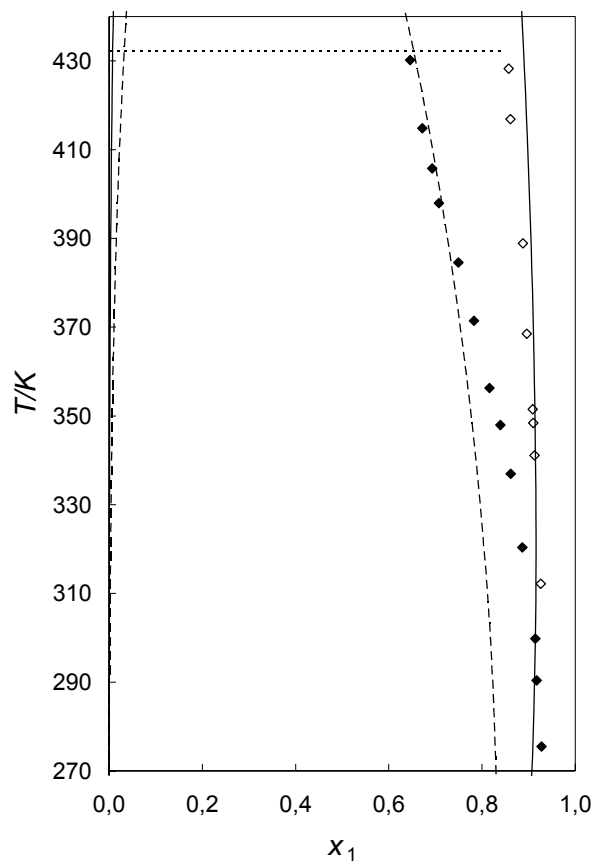


Figure 8S.

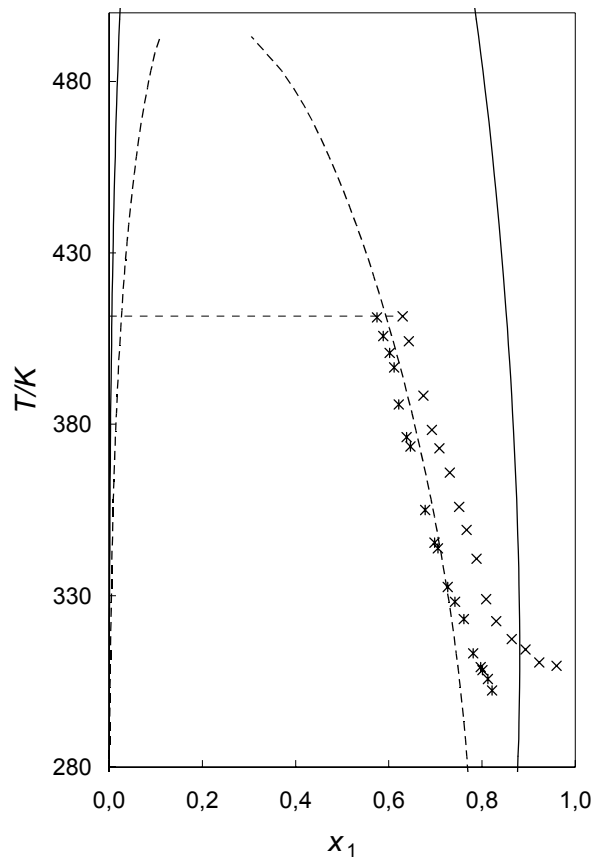


Figure 9S.