**Supplementary Table 3.** Name and Structure of Ionic Liquids

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| No. | Name | Formula | No. Data | Mw | *T* range | *Cp*range | Use as |
| 1 | 1-Butyl-3-methylimidazolium hexafluorophosphate | C8H15F6N2P | 1633 | 284.18 | 283.15-524.87 | 367.3-510 | Training |
| 2 | 1-Hexyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide | C12H19F6N3O4S2 | 502 | 447.42 | 188.06-425.15 | 572-739 | Training |
| 3 | 1-Ethyl-3-methylimidazolium ethyl sulfate | C8H16N2O4S | 450 | 236.29 | 187.36-377.2 | 347-570 | Training |
| 4 | 1-Butyl-3-methylimidazolium tetrafluoroborate | C8H15BF4N2 | 374 | 226.02 | 181.25-423.15 | 276.1-520 | Validation |
| 5 | 1-Methyl-3-propylimidazolium bromide | C7H13BrN2 | 261 | 205.1 | 212.2-370 | 256.1-307 | Training |
| 6 | 1-Methyl-3-octylimidazolium tetrafluoroborate | C12H23BF4N2 | 246 | 282.13 | 192.85-370 | 463.2-544.2 | Training |

**SupplementaryTable 3.**Continued

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| --- | --- | --- | --- | --- | --- | --- | --- |
| 7 | 1-Ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide | C8H11F6N3O4S2 | 178 | 391.31 | 256.91-463.15 | 456-559 | Training |
| 8 | 1-Butyl-3-methylimidazolium dicyanamide | C10H15N5 | 156 | 205.26 | 235-372.2 | 355.9-413.6 | Training |
| 9 | 1-Butyl-3-methylimidazolium trifluoromethanesulfonate | C9H15F3N2O3S | 152 | 288.29 | 290.98-425.15 | 417.2-506 | Training |
| 10 | Trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]imide | C34H68F6NO4PS2 | 150 | 764 | 293-463.15 | 1360-1570 | Training |
| 11 | Trihexyl(tetradecyl)phosphonium tris(pentafluoroethyl)trifluorophosphate | C38H68F18P2 | 143 | 928.87 | 338.15-513.15 | 1540-1810 | Training |
| 12 | 1-Butyl-3-methylimidazolium iodide | C8H15IN2 | 134 | 266.12 | 209.86-370 | 285.8-336.9 | Training |
| 13 | 1-Butyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide | C10H15F6N3O4S2 | 123 | 419.36 | 190-363.18 | 524-602.1 | Training |
| 14 | 1-Hexyl-3-methylimidazolium trifluoromethanesulfonate | C11H19F3N2O3S | 112 | 316.34 | 283.15-425.15 | 484-589 | Training |
| 15 | 2-Hydroxy-N-methylethanaminium propionate | C6H15NO3 | 111 | 149.19 | 287.15-326.15 | 323-336 | Training |
| 16 | 2-Hydroxy-N-methylethanaminium pentanoate | C8H19NO3 | 107 | 177.24 | 283.15-333.15 | 385-421 | Training |
| 17 | N-methyl-2-hydroxyethylammonium butanoate | C7H17NO3 | 92 | 163.21 | 286.15-336.15 | 357-385 | Training |
| 18 | 1-Ethyl-3-methylimidazolium trifluoromethanesulfonate | C7H11F3N2O3S | 76 | 260.23 | 303.2-425.15 | 379-425 | Training |
| 19 | 4-(Dimethylamino)-1-hexyl-pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide | C15H23F6N3O4S2 | 73 | 487.48 | 298-425.15 | 663-825 | Training |
| 20 | n-butyl-4-(n',n'-dimethylammonium)pyridinium bis(trifluoromethylsulfonyl)imid | C13H19F6N3O4S2 | 73 | 459.43 | 298-425.15 | 611-739 | Training |

**Supplementary Table 3.**Continued

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| --- | --- | --- | --- | --- | --- | --- | --- |
| 21 | 1-Octyl-3-methylimidazolium trifluoromethanesulfonate | C13H23F3N2O3S | 64 | 344.39 | 313.17-425.15 | 588-680 | Training |
| 22 | n-ethyl-4-(n',n'-dimethylammonium)pyridinium bis(trifluoromethylsulfonyl)imide | C11H15F6N3O4S2 | 64 | 431.37 | 313.12-425.15 | 590-659 | Training |
| 23 | 1-Butylpyridinium tetrafluoroborate | C9H14BF4N | 63 | 223.02 | 284.33-390 | 377.19-428.5 | Training |
| 24 | Tetradecyl(trihexyl)phosphonium dicyanamide | C34H68N3P | 63 | 549.9 | 313.15-413.15 | 1060-1240 | Training |
| 25 | 1-Butyl-1-methylpyrrolidinium bis[(trifluoromethyl)sulfonyl]imide | C11H20F6N2O4S2 | 61 | 422.41 | 237.44-347.44 | 546.8-622.4 | Validation |
| 26 | 1-Butylpyridinium bis[(trifluoromethyl)sulfonyl]imide | C11H14F6N2O4S2 | 60 | 416.36 | 323.18-425.15 | 587-645 | Training |
| 27 | 3-Methyl-1-propyl-1H-imidazolium (S)-2-amino-4-carboxybutanoate | C12H21N3O4 | 58 | 271.31 | 244.25-357.7 | 471-568.1 | Training |
| 28 | 1-Methyl-1-propylpyrrolidinium bis[(trifluoromethyl)sulfonyl]imide | C10H18F6N2O4S2 | 57 | 408.38 | 283.15-358.15 | 541-606 | Training |
| 29 | 1-Hexyl-3-methylimidazolium hexafluorophosphate | C10H19F6N2P | 51 | 312.24 | 293.15-343.15 | 422-452 | Training |
| 30 | Tributylmethylphosphoniummethylsulphate | C14H33O4PS | 50 | 328.45 | 343.15-463.15 | 661-757 | Training |
| 31 | 1-Tetradecyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide | C20H35F6N3O4S2 | 50 | 559.63 | 309.98-368.07 | 896.3-953.3 | Training |
| 32 | N-(2-hydroxyethyl)-N,N-dimethylpropanaminium bromide | C7H18BrNO | 48 | 212.13 | 382.5-429.98 | 370.7-392.6 | Training |
| 33 | Butyltrimethylammonium bis(trifluoromethylsulfonyl)imide | C9H18F6N2O4S2 | 48 | 396.37 | 278.32-367.93 | 547.5-600.9 | Training |
| 34 | 1-Butyl-3-methylimidazolium octyl sulfate | C16H32N2O4S | 46 | 348.5 | 298.15-343.15 | 635-698 | Training |

**Supplementary Table 3.**Continued

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| --- | --- | --- | --- | --- | --- | --- | --- |
| 35 | 1-Ethyl-3-methylimidazolium tetrafluoroborate | C6H11BF4N2 | 44 | 197.97 | 283.15-358.2 | 303.2-330.7 | Training |
| 36 | 1-Butyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide | C12H16F6N2O4S2 | 43 | 430.39 | 293.1-333.1 | 541-641 | Training |
| 37 | 1-Methyl-3-propylimidazolium bis[(trifluoromethyl)sulfonyl]imide | C9H13F6N3O4S2 | 42 | 405.34 | 293.15-333.15 | 482-534.9 | Training |
| 38 | 1-Ethyl-3-methyl-1H-imidazolium tricyanomethanide | C10H11N5 | 40 | 201.23 | 296.2-372.2 | 357-403.1 | Training |
| 39 | 1-Hexyl-3-methylimidazolium tetrafluoroborate | C10H19BF4N2 | 33 | 254.08 | 283.15-323.15 | 416-444 | Training |
| 40 | 1-Octyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide | C14H23F6N3O4S2 | 33 | 475.47 | 292-372.66 | 690-825 | Training |
| 41 | 1-n-butyl-3-methylimidazolium bromide | C8H15BrN2 | 25 | 219.12 | 225.62-370 | 289-340.9 | Validation |
| 42 | 1-Propylpyridinium tetrafluoroborate | C8H12BF4N | 25 | 208.99 | 278.15-338.15 | 352-385 | Validation |
| 43 | 1-Ethyl-2-methylpyridinium bis((trifluoromethyl)sulfonyl)amide | C10H12F6N2O4S2 | 25 | 402.33 | 278.15-338.15 | 523-553 | Training |
| 44 | 2-Methyl-1-propylpyridinium bis((trifluoromethyl)sulfonyl)imide | C11H14F6N2O4S2 | 25 | 416.36 | 278.15-338.15 | 546-578 | Training |
| 45 | 1-Methyl-1-propylpiperidinium bis(trifluoromethylsulfonyl)imide | C11H20F6N2O4S2 | 24 | 422.41 | 298-520 | 607-756 | Training |
| 46 | 1-Butyl-3-methylimidazolium methylsulfate | C9H18N2O4S | 21 | 250.32 | 283.1-318.15 | 226.1-425.6 | Training |
| 47 | 1-Ethyl-3-methylimidazolium dicyanamide | C8H11N5 | 21 | 177.21 | 296.2-372.2 | 314.6-376.7 | Training |
| 48 | 1-Ethylpyridinium bis[(trifluoromethyl)sulfonyl]imide | C9H10F6N2O4S2 | 21 | 388.31 | 288.15-338.15 | 519-539 | Training |
| 49 | 1-Butyl-3-methylimidazolium acetate | C10H18N2O2 | 21 | 198.26 | 253.15-413.15 | 360-470 | Training |
| 50 | 1-Ethyl-4-methylpyridinium bis((trifluoromethyl)sulfonyl)amide | C10H12F6N2O4S2 | 20 | 402.33 | 296.2-372.2 | 627-715 | Training |

**Supplementary Table 3.**Continued

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| --- | --- | --- | --- | --- | --- | --- | --- |
| 51 | 1-Butyl-4-methylpyridinium bis((trifluoromethyl)sulfonyl)amide | C12H16F6N2O4S2 | 20 | 430.39 | 296.2-372.2 | 636-724 | Training |
| 52 | 1-Ethyl-3-methyl-1H-imidazolium 1,1,2,2-tetrafluoroethane-1-sulfonate | C8H12F4N2O3S | 20 | 292.25 | 296.2-372.2 | 483-563 | Training |
| 53 | N-(2-hydroxyethyl)-N,N-dimethylbutanaminium bromide | C8H20BrNO | 19 | 226.15 | 409.71-438.26 | 382.5-407 | Training |
| 54 | 1-Ethyl-3-methylimidazolium bromide | C6H11BrN2 | 17 | 191.07 | 298-370 | 247-272.6 | Training |
| 55 | 1-Ethyl-3-methylimidazolium diethylphosphate | C10H21N2O4P | 17 | 264.26 | 283.15-343.15 | 460-557 | Training |
| 56 | 1-Butyl-3-methylimidazolium chloride | C8H15ClN2 | 16 | 174.67 | 298-403.2 | 317-376.8 | Training |
| 57 | N-ethyl-N-(2-hydroxyethyl)-N,N-dimethylammonium ethyl sulfate | C8H21NO5S | 16 | 243.32 | 300.15-375.15 | 451-507 | Training |
| 58 | Trihexyltetradecylphosphonium bis(2,4,4-trimethylpentyl)phosphinate | C48H102O2P2 | 15 | 773.27 | 293.15-363.15 | 1619-1764 | Validation |
| 59 | 1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate | C15H20F18NP | 14 | 587.27 | 293-358 | 767-812 | Training |
| 60 | 1-Propylpyridinium hexafluorophosphate | C8H12F6NP | 13 | 267.15 | 377.7-400 | 404-454.3 | Training |
| 61 | N-(2-hydroxyethyl)-N,N-dimethylhexan-1-aminium bromide | C10H24BrNO | 13 | 254.21 | 386.41-403.35 | 465-475 | Training |
| 62 | 1-Butyl-3-methylimidazolium thiocyanate | C9H15N3S | 12 | 197.3 | 296.2-340.2 | 383-421.8 | Validation |
| 63 | 1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy) ethylsulfate | C11H22N2O6S | 12 | 310.37 | 303.2-358.2 | 526-544 | Training |
| 64 | 4,6-Dimethyl-N-phenylpyrimidin-2-amine dodecanoate | C24H37N3O2 | 10 | 399.57 | 323.46-339.25 | 830.6-872.9 | Training |
| 65 | 1-Ethyl-3-methylimidazolium thiocyanate | C7H11N3S | 9 | 169.25 | 283.15-343.15 | 281.4-340.7 | Training |
| 66 | 1-Butyl-3-methyl-1H-imidazolium tetrachloroferrate(III) | C8H15Cl4FeN2 | 9 | 336.88 | 383.17-423.22 | 466-471 | Training |

**Supplementary Table 3.**Continued

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| 67 | N,N-dibutyl-N-methylbutanaminium L-serinate | C16H36N2O3 | 9 | 304.47 | 293.15-363.15 | 632-681 | Validation |
| 68 | N,N-dibutyl-N-methyl-1-butanaminium L-lysinate | C19H43N3O2 | 9 | 345.56 | 293.15-363.15 | 817-925 | Training |
| 69 | N,N-dibutyl-N-methyl-1-butanaminium L-threoninate | C17H38N2O3 | 9 | 318.5 | 293.15-363.15 | 748-821 | Training |
| 70 | Tetrabutylphosphonium L-serinate | C19H42NO3P | 9 | 363.52 | 293.15-363.15 | 742-815 | Training |
| 71 | Tetrabutylphosphonium L-lysinate | C22H49N2O2P | 9 | 404.61 | 293.15-363.15 | 990-1110 | Training |
| 72 | Tetrabutylphosphonium L-threoninate | C20H44NO3P | 9 | 377.54 | 293.15-363.15 | 952-1100 | Training |
| 73 | Tetrabutylphosphonium L-prolinate | C21H44NO2P | 9 | 373.55 | 293.15-363.15 | 838-939 | Training |
| 74 | N,N-dibutyl-N-methyl-1-butanaminium 2-aminoethanesulfonate | C15H36N2O3S | 9 | 324.52 | 293.15-363.15 | 822-892 | Training |
| 75 | Tetrabutylphosphonium L-cysteinate | C19H42NO2PS | 9 | 379.58 | 293.15-363.15 | 914-1020 | Training |
| 76 | N-ethyl-2-hydroxy-N,N-dimethylethanaminium methanesulfonate | C7H19NO4S | 9 | 213.3 | 355.15-395.15 | 406-435 | Training |
| 77 | 2-Hydroxy-N,N,N-trimethyl-ethanaminium 1-butanesulfonate | C9H23NO4S | 9 | 241.35 | 360.15-400.15 | 518-529 | Training |
| 78 | N,N,N-trimethyl-1-butanaminium 1-butanesulfonate | C11H27NO3S | 9 | 253.4 | 360.15-400.15 | 701-741 | Training |
| 79 | 1-Ethyl-3-methylimidazolium tetracyanoborate | C10H11BN6 | 9 | 226.05 | 293.15-363.15 | 406.4-424.3 | Training |
| 80 | 1-Ethyl-3-methylimidazolium methanesulfonate | C7H14N2O3S | 8 | 206.26 | 283.15-343.15 | 327-350 | Training |
| 81 | 1H-imidazolium, 1-ethyl-3-methyl-, salt with trifluoroacetic acid (1:1) | C8H11F3N2O2 | 7 | 224.18 | 283.15-343.15 | 308-337 | Training |
| 82 | 1-(2-hydroxyethyl)-3-methyl-1H-imidazolium 2,2,2-trifluoroacetate | C8H11F3N2O3 | 7 | 240.18 | 283.15-343.15 | 362-394 | Training |
| 83 | 1-ethyl-3-methylimidazolium hydrogen sulfate | C6H12N2O4S | 7 | 208.24 | 283.15-343.15 | 290-324 | Training |

**Supplementary Table 3.**Continued

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| 84 | tributylethylphosphonium diethylphosphate | C18H42O4P2 | 7 | 384.47 | 283.15-343.15 | 683-768 | Training |
| 85 | 1-Methyl-3-octylimidazolium L-asparaginate | C16H30N4O3 | 7 | 326.43 | 293.1-353.1 | 654-717 | Training |
| 86 | 1-Methyl-3-octylimidazolium L-alaninate | C15H29N3O2 | 7 | 283.41 | 293.1-353.1 | 592-657 | Training |
| 87 | 1-Methyl-3-octyl-1H-imidazol-3-ium L-prolinate | C17H31N3O2 | 7 | 309.45 | 293.1-353.1 | 562-628 | Training |
| 88 | N-ethyl-N,N-dimethyl-N-butylammonium ethyl sulfate | C10H25NO4S | 7 | 255.37 | 360.15-390.15 | 451-500 | Training |
| 89 | 1-Ethyl-3-methylimidazolium tosylate | C13H18N2O3S | 6 | 282.36 | 318.15-368.15 | 484.2-599 | Training |
| 90 | 1,3-Dimethylimidazolium methylsulfate | C6H12N2O4S | 6 | 208.24 | 318.15-368.15 | 340.7-396.1 | Training |
| 91 | Tetrapropylammonium bromide | C12H28BrN | 6 | 266.26 | 283.01-348.43 | 333-393 | Training |
| 92 | Pyrrolidinium nitrate | C4H10N2O3 | 5 | 134.13 | 298.15-318.15 | 227-229 | Validation |
| 93 | 1-Ethylpyridinium hexafluorophosphate | C7H10F6NP | 5 | 253.13 | 380-400 | 379.6-389.6 | Training |
| 94 | 1-Butyl-3-methylimidazolium tosylate | C15H22N2O3S | 5 | 310.41 | 343.89-380 | 543.4-569.8 | Training |
| 95 | 1-Ethyl-3-methylimidazolium methylsulfate | C7H14N2O4S | 4 | 222.26 | 288.15-343.15 | 331-354 | Validation |
| 96 | 1,2-Dimethyl-3-propylimidazolium bis[(trifluoromethyl)sulfonyl]imide | C10H15F6N3O4S2 | 3 | 419.36 | 298.15-323.15 | 470-559 | Training |
| 97 | 3-Hexyl-1-methyl-1H-imidazolium bromide | C10H19BrN2 | 3 | 247.18 | 298-323 | 344-376 | Training |
| 98 | 3-Cyano-1-octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide | C16H21F6N3O4S2 | 3 | 497.48 | 298.15-353.15 | 709-731 | Training |
| 99 | 1-Hexyl-4-cyanopyridinium bis(trifluoromethylsulfonyl)imide | C14H17F6N3O4S2 | 3 | 469.42 | 298.15-353.15 | 633-652 | Training |
| 100 | 1-Butyl-3-cyanopyridinium bis(trifluoromethylsulfonyl)imide | C12H13F6N3O4S2 | 3 | 441.37 | 298.15-353.15 | 586-605 | Training |
| 101 | 3-Cyano-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide | C14H17F6N3O4S2 | 3 | 469.42 | 298.15-353.15 | 658-681 | Training |

**Supplementary Table 3.**Continued

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| 102 | 1-Methylpyridinium methylsulfate | C7H11NO4S | 3 | 205.23 | 288.15-308.15 | 288-305 | Training |
| 103 | 1,2-Diethylpyridinium ethylsulfate | C11H19NO4S | 3 | 261.34 | 288.15-308.15 | 399-420 | Training |
| 104 | 1-Butyl-1-methylpyrrolidinium trifluoromethanesulfonate | C10H20F3NO3S | 3 | 291.33 | 288.15-308.15 | 424-441 | Training |
| 105 | 3-(Ethoxycarbonyl)-1-ethylpyridinium ethylsulfate | C12H19NO6S | 2 | 305.35 | 298-323 | 513-530 | Training |
| 106 | 1-Ethyl-3-methylpyridinium ethylsulfate | C10H17NO4S | 2 | 247.31 | 298-323 | 389-402 | Training |
| 107 | 17-Hydroxy-N-(17-hydroxy-3,6,9,12,15-pentaoxaheptadec-1-yl)-N-methyl-N-tetradecyl-3,6,9,12,15-pentaoxaheptadecan-1-aminium methyl sulfate | C40H85NO16S | 2 | 868.16 | 298-323 | 1070-1100 | Training |
| 108 | Tetrabutylammonium docusate | C36H73NO7S | 2 | 664.03 | 298-323 | 1320-1380 | Training |
| 109 | 1-methyl-3-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-1H-imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide | C12H12F15N3O4S2 | 2 | 611.35 | 298-323 | 725-752 | Training |
| 110 | 1-Hexyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide | C13H21F6N3O4S2 | 2 | 461.44 | 298-323 | 686-705 | Training |
| 111 | 1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate | C13H26N2O6S | 2 | 338.42 | 298-323 | 643-652 | Training |
| 112 | 1-Octyl-3-methylpydridinium bis(trifluoromethylsulfonyl)imide | C16H24F6N2O4S2 | 2 | 486.49 | 298-323 | 669-693 | Training |
| 113 | 1-Hexyl-3-methyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide | C16H25F6N3O4S2 | 2 | 501.51 | 298-323 | 725-764 | Training |

**Supplementary Table 3.**Continued

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| 114 | 1-Hexyl-4-(4-methyl-1-piperidinyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide | C19H29F6N3O4S2 | 2 | 541.57 | 298-323 | 628-650 | Training |
| 115 | 1-Butyl-3-methylpyridinium tetrafluoroborate | C10H16BF4N | 2 | 237.05 | 298-323 | 405-421 | Training |
| 116 | 1-Butyl-nicotinic acid butyl ester bis[(trifluoromethyl)sulfonyl]imide | C16H22F6N2O6S2 | 2 | 516.48 | 298-323 | 707-727 | Training |
| 117 | 1-Hexylpyridinium bis(trifluromethylsulfonyl)imide | C13H18F6N2O4S2 | 2 | 444.41 | 298-323 | 612-632 | Training |
| 118 | 1-Hexyl-3-methylpyridinium bromide | C12H20BrN | 2 | 258.2 | 298-323 | 343-358 | Training |
| 119 | 1-Hexyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide | C14H20F6N2O4S2 | 2 | 458.44 | 298-323 | 624-644 | Training |
| 120 | 1-Hexyl-3,5-dimethylpyridinium bis(trifluoromethylsulfonyl)imide | C15H22F6N2O4S2 | 2 | 472.47 | 298-323 | 620-665 | Training |
| 121 | 3,5-Diethyl-1-hexyl-2-propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide | C20H32F6N2O4S2 | 2 | 542.6 | 298-323 | 766-799 | Training |
| 122 | 1-Butyl-2,3-dimethylimidazolium tetrafluoroborate | C9H17BF4N2 | 2 | 240.05 | 330.15-372.15 | 375.3-406.5 | Training |
| 123 | 1-Ethyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide | C9H13F6N3O4S2 | 2 | 405.34 | 309.15-323.15 | 492.7-499 | Training |
| 124 | 1-Butyl-2,3-dimethylimidazolium hexafluorophosphate | C9H17F6N2P | 2 | 298.21 | 298.15-323.15 | 433.6-449.1 | Training |
| 125 | 1-Butyl-3-methylpyridinium tetracyanoborate | C14H16BN5 | 2 | 265.12 | 298.15-323.15 | 495-524 | Validation |
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**Supplementary Table 3.**Continued

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| 126 | 1-Butyl-1-methylpyrrolidinium tetracyanoborate | C13H20BN5 | 2 | 257.14 | 298.15-323.15 | 524-554 | Training |
| 127 | 1-Butyl-3-methylpyridinium tricyanomethanide | C14H16N4 | 2 | 240.3 | 298.15-323.15 | 468-479 | Training |
| 128 | 1-Methyl-3-octylimidazolium bromide | C12H23BrN2 | 1 | 275.23 | 298 | 440 | Training |
| 129 | N-butyl-3-methylpyridinium dicyanamide | C12H16N4 | 1 | 216.28 | 298.15 | 368 | Training |
| 130 | 3-(2-Hydroxyethyl)-1-methyl-1H-imidazol-3-ium dicyanoazanide | C8H11N5O | 1 | 193.21 | 298.15 | 231.8 | Training |
| 131 | 1-Butyl-3-methylimidazolium tricyanomethane | C12H15N5 | 1 | 229.28 | 298.15 | 298.1 | Training |
| 132 | 1-Ethyl-3-methylimidazolium acetate | C8H14N2O2 | 1 | 170.21 | 298.15 | 321.9 | Training |
| 133 | 1-Ethyl-3-methylimidazolium dimethylphosphate | C8H17N2O4P | 1 | 236.21 | 298.15 | 412 | Training |
| 134 | 1-Ethyl-3-methylimidazolium methyl phosphonate | C7H15N2O3P | 1 | 206.18 | 298.15 | 355 | Training |
| 135 | 1-Pentyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide | C11H17F6N3O4S2 | 1 | 433.39 | 298.15 | 595.6 | Training |
| 136 | 1-Heptyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide | C13H21F6N3O4S2 | 1 | 461.44 | 298.15 | 659.2 | Training |
| 137 | 1-Dodecyl-3-methyl-1H-imidazolium bis(trifluoromethylsulfonyl)amide | C18H31F6N3O4S2 | 1 | 531.58 | 298.15 | 820.2 | Training |
| 138 | 1-Decyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide | C16H27F6N3O4S2 | 1 | 503.52 | 298.15 | 754.5 | Training |
| 139 | 1-Hexyl-3-methylimidazolium chloride | C10H19ClN2 | 1 | 202.72 | 298 | 381 | Training |
| 140 | 1-Methyl-3-octylimidazolium chloride | C12H23ClN2 | 1 | 230.78 | 298 | 445 | Training |
| 141 | 1,3-Dimethylimidazolium bromide | C5H9BrN2 | 1 | 177.04 | 298 | 215 | Training |