CHEMPHYSCHEM

Supporting Information

Anion and cation effects on imidazolium salt melting points: A descriptor modelling study

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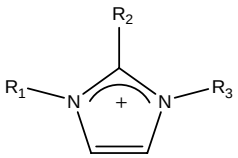
Table 1. Descriptor values for the 1-ethyl-3-methylimidazolium salts.

Entry	Anion	Y_{index}	X_3A	X_5sol	STN	SRW05	SRW06	G_m	PW_5	RNCG
1	Trifluoro-*N*-(trifluoromethylsulfonyl)acetamide	2.762	0.216	0	0	0	566	0.208	0.047	0.260
2	Bis{(pentafluoroethyl)sulfonyl}amide	2.885	0.191	0.497	0	0	1024	0.570	0.031	0.228
3	Bis{(trifluoromethyl)sulfonyl}amide	3.001	0.206	0	0	0	664	0.324	0.046	0.253
4	Bis(1,2-benzenediolato(2-)-*O,O'*)-borate	0.816	0.165	5.403	6.735	20	772	1	0.119	0.105
5	Pentafluorethylsulfonate	4.268	0.208	0	0	0	488	0.331	0	0.241
6	Methylsulfate	5.184	0.354	0	0	0	160	0.386	0	0.273
7	Trifluoromethanesulfonate	4.976	0.250	0	0	0	308	0.321	0	0.265
8	Nonafluorobutyltrifluoroborate	3.667	0.191	0	0	0	848	0.209	0.036	0.122
9	Heptafluoropropyltrifluoroborate	3.902	0.197	0	0	0	668	0.208	0.028	0.137
10	Pentafluoroethyltrifluoroborate	4.268	0.208	0	0	0	488	0.256	0	0.155
11	Trifluoromethyltrifluoroborate	4.976	0.250	0	0	0	308	0.321	0	0.182
12	Trifluoroethanoate	4.656	0.289	0	0	0	216	0.341	0	0.304
13	Tetrachloroaluminate(III)	0	0	0	0	0	128	1	0	0.250
14	Bis(oxalate(2-)-borate	1.402	0.177	2.856	3.219	20	556	1	0.097	0.134
15	Bis(trifluoromethyl)imide	3.164	0.177	0	0	0	304	0.432	0	0.297
16	Dicyanamide	2.340	0.354	0	0	0	56	0.670	0	0.355
17	Tricyanomethanide	2.933	0.289	0	0	0	132	0.693	0	0.320
18	Tosylate	1.648	0.203	1.912	1.792	0	394	0.311	0.066	0.234
19	Nitrate	0	0	0	0	0	54	0.794	0	0.333
20	Nitrite	0	0	0	0	0	16	0.729	0	0.500
21	Tetrafluoroborate	0	0	0	0	0	128	1	0	0.250
22	Perchlorate	0	0	0	0	0	128	1	0	0.250

Table 2. Anion sphericity values for the second dataset.

Entry	Anion	Sphericity
1	Tetrachloroaluminate	0.75
2	Hexafluorophosphate(V)	0.83
3	Nitrate	0.67
4	Tetrafluroborate	0.75
5	Nitrite	0.50
6	Hexafluoroantimonate(V)	0.83
7	Perchlorate	0.75
8	Hexafluoroarseniate(V)	0.83
9	Chloride	1
10	Bromide	1
11	Iodide	1

Table 3. Cation Decriptor Values for the second dataset.

Entry	Cation 			PW_2	MSD	RDF40	RDF55	RDF125
	R_1	R_2	R_3					
1	Me	Me	Et	0.575	0.302	13.421	4.609	0.000
2	Me	Me	^{n}Pr	0.561	0.312	13.389	6.824	0.000
3	Me	Me	^{n}Bu	0.555	0.323	13.444	8.780	0.000
4	Me	H	Me	0.571	0.328	5.257	3.284	0.000
5	Me	H	Et	0.554	0.334	4.660	5.207	0.000
6	Me	H	^{n}Pr	0.541	0.344	7.252	6.688	0.000
7	Me	H	Allyl	0.541	0.344	4.743	6.160	0.000
8	Me	H	^{n}Bu	0.537	0.354	6.934	6.978	0.000
9	Me	H	Pentyl	0.533	0.363	7.804	8.942	0.000
10	Me	H	Hexyl	0.531	0.370	8.462	11.903	0.000
11	Me	H	Heptyl	0.528	0.377	9.250	10.607	0.000
12	Me	H	Octyl	0.526	0.382	9.982	11.599	0.404
13	Me	H	Nonyl	0.524	0.386	9.508	11.810	1.567
14	Me	H	Decyl	0.523	0.389	10.180	11.962	8.471
15	Me	H	Undecyl	0.522	0.392	10.606	12.087	9.543
16	Me	H	Dodecyl	0.520	0.395	11.118	12.383	9.842
17	Me	H	Tridecyl	0.519	0.397	11.675	12.653	10.539
18	Me	H	Tetradecyl	0.518	0.399	12.212	12.787	11.157
19	Me	H	Pentadecyl	0.517	0.400	12.577	13.075	11.882
20	Me	H	Hexadecyl	0.517	0.402	13.077	13.165	12.647
21	Me	H	Octadecyl	0.515	0.404	14.127	13.709	14.047
22	H	H	Me	0.544	0.340	2.677	0.077	0.000