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Supporting Information Table S1 Correlation of the melting point of the imidazolium bromides (Set A) by Heuristic Method

P	R^2	F	S^2		B	ΔB	t	Name of descriptor
1	0.2819	21.59	2220.4	0	-247.24	89.24	-2.77	Intercept
				1	244.7	52.66	4.65	Internal heat/number of atoms
2	0.4955	26.52	1588.7	0	6342.1	972.02	6.52	Intercept
				1	-1151.8	181.98	-6.33	Maximum exchange energy for a C-H bond
				2	-696.56	134.14	-5.19	Moment of inertia
3	0.6316	30.29	1182.1	0	5457.0	841.4	6.49	Intercept
				1	-1096.9	153.8	-7.13	Maximum exchange energy for a C-H bond
				2	33.28	5.34	6.23	HOMO energy
				3	1346.9	267.7	5.03	Minimum atomic orbital electronic population
4	0.6862	28.42	1026.4	0	3377.3	733.2	4.61	Intercept
				1	-47.95	5.96	-8.05	HOMO-LUMO energy gap
				2	1471.6	252.2	5.84	Minimum atomic orbital electronic population
				3	-4070.9	751.8	-5.42	Maximum SIGMA-SIGMA bond order
				4	0.3599	0.1108	3.25	Final heat of formation
5	0.7442	29.67	853.1	0	944.8	355.7	2.66	Intercept
				1	-62.02	6.16	-10.1	HOMO-LUMO energy gap
				2	96.58	14.68	6.58	Balaban index
				3	1482.1	232.1	6.39	Minimum atomic orbital electronic population
				4	667.4	141.7	4.71	Maximum partial charge for a N atom
				5	-8.168	1.89	-4.32	Maximum e-n attraction for a C atom

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Supporting Information Table S2 Correlation of the melting point of the imidazolium bromides (Set B) by Heuristic Method

P	R^2	F	S^2		B	ΔB	t	Name of descriptor
1	0.3896	17.24	439.71	0	127.82	7.92	16.14	Intercept
				1	50.52	12.17	4.15	Total hybridization component of the molecular dipole
2	0.4791	11.96	389.72	0	100.3	13.6	7.36	Intercept
				1	6.23	1.34	4.64	HACA-1 [Zefirov's PC]
				2	36.66	1.08	3.39	Average complementary information content of the order 2
3	0.6532	15.69	269.86	0	3052.8	658.2	4.64	Intercept
				1	0.923	0.154	5.98	HASA-1 [Zefirov's PC]
				2	-9.26	2.07	-4.49	Maximum e-n attraction for a C-N bond
				3	9.22	2.27	4.05	WPSA-3 Weighted PPSA (PPSA3*TMSA/1000)
4	0.7040	14.27	239.90	0	1841.3	313.3	5.88	Intercept
				1	1.021	0.154	6.64	HASA-1 [Zefirov's PC]
				2	-9.923	1.891	-5.25	Maximum e-e repulsion for a C-N bond
				3	-417.4	88.9	-4.70	RPCG Relative positive charge
				4	-115.3	48.8	-2.36	XY Shadow / XY Rectangle
5	0.7517	13.93	209.96	0	4513.1	654.6	6.89	Intercept
				1	-14.04	2.07	-6.78	Maximum e-n attraction for a C-N bond
				2	0.905	0.138	6.56	HA dependent HDSA-1 [Zefirov's PC]
				3	3.69	0.71	5.23	Number of H atoms
				4	51.16	15.02	3.41	Image of the Onsager-Kirkwood solvation energy
				5	-341.5	122.2	-2.79	Maximum partial charge for a O atom [Zefirov's PC]

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Supporting Information Table S3 Correlation of the melting point of the (Set C) by Heuristic Method

P	R^2	F	S^2		B	ΔB	t	Name of descriptor
1	0.5805	22.14	2022.47	0	1694.2	319.86	5.30	Intercept
				1	14189	3015.4	4.71	Maximum partial charge for a N atom
2	0.8580	45.32	730.22	0	3091.6	379.44	8.15	Intercept
				1	-2730.1	347.37	-7.86	Average bond order of a N atom
				2	3135.7	451.15	6.95	Maximum partial charge for a C atom
3	0.9432	77.53	312.80	0	3026.7	426.1	7.10	Intercept
				1	25.78	1.82	14.16	RNCS Relative negative charged SA (SAMNEG*RNCG) [Zefirov's PC]
				2	4.52	0.36	12.42	HA dependent HDSA-1 [Zefirov's PC]
				3	-10.03	1.40	-7.19	Minimum e-n attraction for a C-H bond

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Supporting Information Table S4 Correlation of the melting point of the benzimidazolium bromides (Set D) by Heuristic Method

P	R^2	F	S^2		B	ΔB	t	Name of descriptor
1	0.1763	9.21	935.43	0	822.07	194.30	4.23	Intercept
				1	-150.64	49.65	-3.03	Maximum coulombic interaction for a C-H bond
2	0.4401	16.11	666.43	0	1028.4	171.45	6.00	Intercept
				1	-207.69	44.07	-4.71	Maximum coulombic interaction for a C-H bond
				2	453.81	101.24	4.40	FHDSA Fractional HDSA (HDSA/TMSA)
3	0.5201	14.45	585.46	0	920.19	161.87	5.68	Intercept
				1	-219.21	41.51	-5.28	Maximum coulombic interaction for a C-H bond
				2	0.72	0.17	4.27	HDSA H donors surface area
				3	29.69	10.82	2.75	Minimum exchange energy for a C-C bond
4	0.6219	16.04	473.09	0	880.4	146.0	6.03	Intercept
				1	-221.4	37.3	-5.93	Maximum coulombic interaction for a C-H bond
				2	0.868	0.158	5.48	HDSA H donors surface area [Semi-MO PC]
				3	40.24	10.25	3.93	Minimum exchange energy for a C-C bond
				4	-10.14	3.13	-3.24	RPCS Relative positive charged SA
5	0.6899	16.91	398.28	0	1015.2	141.9	7.15	Intercept
				1	-224.4	34.3	-6.55	Maximum coulombic interaction for a C-H bond
				2	0.737	0.152	4.84	HDSA H-donors surface area [Semi-MO PC]
				3	45.32	9.57	4.74	Minimum exchange energy for a C-C bond
				4	-12.04	2.95	-4.09	RPCS Relative positive charged SA
				5	-1752.2	607.3	-2.89	Maximum electrophilic reactivity index for a C atom

Supporting Information Table S5 Intercorrelations of Descriptors for eq 1

	D1	D2	D3	D4	D5
R^2	0.2603	0.2756	0.0644	0.0280	0.0407

D1 = Balaban index
D2 = HOMO-LUMO energy gap
D3 = Minimum electronic orbital electronic population
D4 = Maximum partial charge for a N atom
D5 = Maximum e-n attraction for a C atom

Supporting Information Table S6 Intercorrelations of Descriptors for eq 2

	D1	D2	D3	D4	D5
R^2	0.3892	0.2905	0.4037	0.3502	0.3361

D1 = HA dependent HDSA-1 [Zefirov's PC]
D2 = Maximum e-n attraction for a C-N bond
D3 = Number of H atoms
D4 = Image of the Onsager-Kirkwood solvation energy
D5 = Maximum partial charge for a O atom

Supporting Information Table S7 Intercorrelations of Descriptors for eq 3

	D1	D2	D3
R^2	0.3149	0.3641	0.2246

D1 = RNCS Relative negative charged SA (SAMNEG*RNCG) [Zefirov's PC]
D2 = HA dependent HDSA-1 [Zefirov's PC]
D3 = Minimum e-n attraction for a C-N bond

Supporting Information Table S8 Intercorrelations of Descriptors for eq 4

	D1	D2	D3	D4	D5
R^2	0.2279	0.0942	0.1764	0.1842	0.2356

D1 = HDSA H-donors surface area [Semi-MO PC]
D2 = Maximum coulombic interaction for a C-H bond
D3 = Minimum exchange energy for a C-C bond
D4 = Maximum electrophilic reactivity index for a C atom
D5 = RPCS Relative positive charged SA

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Supporting Information Table S9 Validation of correlations for eq 1 (set A)

Subsets	R^2	Group referred
I+II	0.6656	III
I+III	0.6375	II
II+III	0.8156	I
Whole set	0.7080	