Supplementary Information

A group contribution approach for predicting the environmental impacts of imidazolium-based ionic liquids

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Table S1 Molecular weight of the ionic liquids sample assessed. The column Type indicated whether a molecule was used for the training and validation of the GC models or used as a test sample.

Ionic liquid	Abbreviation	MW (g/mol)	Type
1-methylimidazolium chloride	[Hmim]Cl	118.56	Test
1-methylimidazolium tetrafluoroborate	[Hmim][BF_4]	169.90	Train/Validation
1-methylimidazolium hexafluorophosphate	[Hmim][PF_6]	228.10	Train/Validation
1-ethyl-3-methylimidazolium chloride	[C_2mim]Cl	146.62	Test
1-ethyl-3-methylimidazolium tetrafluoroborate	[C_2mim][BF_4]	198.00	Train/Validation
1-ethyl-3-methylimidazolium hexafluorophosphate	[C_2mim][PF_6]	256.10	Train/Validation
1-butyl-3-methylimidazolium chloride	[C_4mim]Cl	174.67	Train/Validation
1-butyl-3-methylimidazolium tetrafluoroborate	[C_4mim][BF_4]	226.00	Test
1-butyl-3-methylimidazolium hexafluorophosphate	[C_4mim][PF_6]	284.20	Test
1-hexyl-3-methylimidazolium chloride	[C_6mim]Cl	202.72	Test
1-hexyl-3-methylimidazolium tetrafluoroborate	[C_6mim][BF_4]	254.10	Test
1-hexyl-3-methylimidazolium hexafluorophosphate	[C_6mim][PF_6]	312.20	Train/Validation
1-octyl-3-methylimidazolium chloride	[C_8mim]Cl	230.80	Train/Validation
1-octyl-3-methylimidazolium tetrafluoroborate	[C_8mim][BF_4]	282.13	Train/Validation
1-octyl-3-methylimidazolium hexafluorophosphate	[C_8mim][PF_6]	340.29	Train/Validation
1-decyl-3-methylimidazolium chloride	[C_{10}mim]Cl	258.83	Train/Validation
1-decyl-3-methylimidazolium tetrafluoroborate	[C_{10}mim][BF_4]	310.20	Test
1-decyl-3-methylimidazolium hexafluorophosphate	[C_{10}mim][PF_6]	368.30	Train/Validation
1-allyl-3-methylimidazolium chloride	[Amim]Cl	158.63	Test
1-allyl-3-methylimidazolium tetrafluoroborate	[Amim][BF_4]	210.00	Train/Validation
1-allyl-3-methylimidazolium hexafluorophosphate	[Amim][PF_6]	268.10	Train/Validation
1-benzyl-3-methylimidazolium chloride	[Bzmim]Cl	208.69	Train/Validation
1-benzyl-3-methylimidazolium tetrafluoroborate	[Bzmim][BF_4]	260.00	Test
1-benzyl-3-methylimidazolium hexafluorophosphate	[Bzmim][PF_6]	318.20	Test
1-phenyl-3-methylimidazolium chloride	[Phmim]Cl	194.70	Train/Validation
1-phenyl-3-methylimidazolium tetrafluoroborate	[Phmim][BF_4]	246.07	Train/Validation
1-phenyl-3-methylimidazolium hexafluorophosphate	[Phmim][PF_6]	304.17	Train/Validation
1-butyl-2,3-dimethylimidazolium chloride	[C_4dmim]Cl	188.70	Train/Validation
1-butyl-2,3-dimethylimidazolium tetrafluoroborate	[C_4dmim][BF_4]	240.10	Test
1-butyl-2,3-dimethylimidazolium hexafluorophosphate	[C_4dmim][PF_6]	298.20	Test

Table S2 Physicochemical properties of relevant chemical compounds to this study

Chemical compound	Chemical formula	Molecular weight (g/mol)	Calorific value, Cp (kJ/mol K)	Heat of formation, $\Delta H°f$ (kJ/mol)	Assumptions	Source
1,2-Dimethylimidazole	$C_5H_8N_2$	96.13	0.10509	1.40	Assumed as 2-methylimidazole (solid phase)	[1]
1-Allyl-3-methylimidazolium chloride	$C_7H_{11}ClN_2$	158.63	0.7720	206.2	ΔH*f*° of 1-butyl-3-methylimidazolium dicyanamide used as proxy.	[2]
1-Benzyl-3-methylimidazolium chloride	$C_{11}H_{13}ClN_2$	208.69	0.7720	206.2	ΔH*f*° of 1-butyl-3-methylimidazolium dicyanamide used as proxy.	[2]
1-Butanol	$C_4H_{10}O$	74.10	0.1769	19.00		[1]
1-Butyl-2,3-dimethylimidazolium chloride	$C_9H_{17}ClN_2$	188.70	0.7720	206.2	ΔH*f*° of 1-butyl-3-methylimidazolium dicyanamide used as proxy.	[2]
1-Butyl-3-methylimidazolium chloride	$C_8H_{15}ClN_2$	174.67	0.7720	206.2	ΔH*f*° of 1-butyl-3-methylimidazolium dicyanamide used as proxy.	[2]
1-Decanol	$C_{10}H_{22}O$	158.28	0.3730	-478.10		[1]
1-Decyl-3-methylimidazolium chloride	$C_{14}H_{27}ClN_2$	258.83	0.7720	206.2	ΔH*f*° of 1-butyl-3-methylimidazolium dicyanamide used as proxy.	[2]
1-Ethyl-3-methylimidazolium chloride	$C_6H_{11}ClN_2$	146.62	0.7720	206.2	ΔH*f*° of 1-butyl-3-methylimidazolium dicyanamide used as proxy.	[2]
1-Hexanol	$C_6H_{14}O$	102.16	0.2432	-377.50		[1]
1-Hexyl-3-methylimidazolium chloride	$C_{10}H_{19}ClN_2$	202.72	0.7720	206.2	ΔH*f*° of 1-butyl-3-methylimidazolium dicyanamide used as proxy.	[2]
1H-Imidazole	$C_3H_4N_2$	68.08	0.0824	54.15	Solid phase	[1]
1-Methylimidazole	$C_4H_6N_2$	82.10	0.10509	1.40	Assumed as 2-methylimidazole (solid phase)	[1]
1-Methylimidazolium chloride	$C_4H_6N_2 \cdot HCl$	118.56	0.7720	206.2	ΔH*f*° of 1-butyl-3-methylimidazolium dicyanamide used as proxy.	[2]
1-Octyl-3-Methylimidazolium chloride	$C_{10}H_{19}ClN_2$	230.80	0.4419	258.94	Δ$H°f$ of 1-octyl-3-methylimidazolium dicyanamide used as proxy.	[3], [4]
1-Phenyl-3-Methylimidazolium chloride	$C_{11}H_{13}ClN_2$	194.70	0.7720	206.2	ΔH*f*° of 1-butyl-3-methylimidazolium dicyanamide used as proxy.	[2], [3]
2-Methylimidazole	$C_4H_6N_2$	82.10	0.10509	1.40	Solid phase	[1]
Acetaldehyde	C_2H_4O	44.05	0.0891	-196.40		[1]
Allyl chloride	C_3H_5Cl	76.53	0.1251	-5.60	Δ$H°f$ is for gas phase	[1]
Ammonia	NH_3	17.03	0.0356	-45.92	Gas phase	[1]
Benzyl chloride	C_7H_7Cl	126.58	0.1824	-33.00		[1]
Butyl chloride	C_4H_9Cl	92.57	0.1594	-188.20		[1]
Chlorine	Cl_2	70.91	0.0339	0.00	Gas phase	[1]

Table S3 Physicochemical properties of relevant chemical compounds to this study (Continued)

Chemical compound	Chemical formula	Molecular weight (g/mol)	Calorific value, Cp (kJ/mol K)	Heat of formation, $\Delta H°f$ (kJ/mol)	Assumptions	Source
Decyl chloride	$C_{10}H_{21}Cl$	176.73	0.3486	-265.47	Cp is calculated at 465 K	[3]
Ethyl chloride	C_2H_5Cl	64.51	0.1088	-137.00		[1]
Ethylene	C_2H_4	28.05	0.0429	52.40	Gas phase	[1]
Formaldehyde	CH_2O	30.03	0.0354	-112.25	Gas phase	[1]
Glyoxal	$C_2H_2O_2$	58.04	0.0602	-212.00	Gas phase	[1]
Hexyl chloride	$C_6H_{13}Cl$	120.62	0.2162	-182.91	Gas phase	[3]
Hydrochloric acid	HCl	36.46	0.0291	-92.31	Gas phase	[1]
Lithium chloride	LiCl	42.39	0.0480	-390.76		[1]
Lithium hexafluorophosphate	$LiPF_6$	151.91	0.1511	-2296.00		[5]
Methanol	CH_4O	32.04	0.0795	-238.40		[1]
Methyl chloride	CH_3Cl	50.49	0.0812	-102.4		[1]
Octyl chloride	$C_8H_{17}Cl$	148.67	0.2747	-238.9	$\Delta H°f$ gas phase	[1]
Phenyl chloride	C_6H_5Cl	112.56	0.1521	11.5	$\Delta H°f$ liquid phase	[1]
Propylene	C_3H_6	42.08	0.1020	20.41	$\Delta H°f$ gas phase	[1]
Sodium chloride	NaCl	58.43	0.0505	-385.92		[1]
Sodium tetrafluoroborate	BF_4Na	109.79	0.1166	-1845.00		[6]
Toluene	C_7H_8	92.14	0.1571	12.00		[1]
Water	H_2O	18.02	0.0754	-285.83		[1]

Sample calculations for estimating the inventory data of an ionic liquid

The inventory data used in this study was obtained using the stoichiometric method at level 3 according to the work of Parvatker and Eckelman [7]. Taking 1-methylimidazoloium chloride, [Hmim]Cl, as an example, the material and energy requirements were estimated following the calculations provided below.

Material requirements

Table S4 Material flow inventory for the imidazole ring formation step.

	Reactants			Products and unreacted material				
	Glyoxal	Ammonia	FA[a]	**1H-Imidazole**	Water	Glyoxal[b]	Ammonia[b]	FA[a,b]
MW (g/mol)	58.04	17.03	30.03	68.1	18	58.04	17.03	30.03
Stoichiometric moles	1	2	1	1	3	-	-	-
Actual moles	1.5	3.0	1.5	1.28	3.9	0.23	0.4	0.14
Grams	87.1	51.1	45	87.1	70.3	13.3	6.8	4.2
Yield (%)	85							

[a] Formaldehyde; [b] Assumed as organic waste stream in Table 2.

Table S5 Material flow inventory for the methylation step.

	Reactants		Products and unreacted material		
	1H-Imidazole	Methyl chloride	**1-methylimidazole chloride**	Imidazole[a]	Methyl chloride[a]
MW (g/mol)	68.1	50.5	118.56	68.1	50.5
Stoichiometric moles	1	1	1	-	-
Actual moles	1.28	1.28	1	0.3	0.3
Grams	87.1	64.7	118.56	19.2	14.2
Yield (%)	76				

[a] Assumed as organic waste stream in Table 2.

Energy requirements

The energy requirements for the production of the 24 ionic liquids sample assessed here were estimated using the heat of formation of the reactants and products, according to the following equations [8]:

$$Q - W = \Delta H + \Delta E_k + \Delta E_p \qquad (S1)$$

where Q is reactor heat consumption, W is the work, ΔH is the enthalpy of reaction, ΔE_k is the kinetic energy, and ΔE_p is the potential energy.

In this case it was assumed that no work is carried and that the kinetic and potential energy are zero, therefore, the heat required by a reactor is equal to the enthalpy of reaction.

$$\Delta H = \sum_{i}^{\text{output streams}} n_i \, \hat{H}_i - \sum_{i}^{\text{input streams}} n_i \, \hat{H}_i \qquad (S2)$$

where n_i is the molecular weight of s i, and H_i is the specific enthalpy of species i given by

$$\hat{H} = \Delta \hat{H}_f^o + \int_{T_1}^{T_2} C_p dT \qquad (S3)$$

where: $\Delta \hat{H}_f^\circ$ is heat of formation of reactants, C_p is the hear capacity, T_1 is the reference absolute temperature (25 ºC), and T_2 is the absolute temperature.

All relevant physico-chemical properties used for these calculations are provided in Table S2, and the specific reaction conditions including temperature of the reactants are reported in Section 2.2 of the paper.

The estimated theoretical energy consumption was scaled-up to industrial scale by multiplying it by the correction factors reported in Mehrkesh and Karunanithi [9]. For heat requirements for endothermic reactions, the estimated theoretical value was converted to the actual heat consumption (assumed to be supplied by natural gas) using a correction factor of 4.2. Similarly, the theoretical heat generated by exothermic reactions was converted to the actual cooling electricity requirements using a correction factor of 3.2.

Sample calculations for 1-methylimidazoloium chloride ([Hmim]Cl) shown below:

1-methylimidazoloium chloride ([Hmim]Cl)

The energy inventory for the production of 118.56 g (1 mol) of [Hmim]Cl has been estimated based on the heat requirements of the reactor using eqns. (S1)–(S3). Table S5 shows the input and output streams involved in the synthesis of [Hmim]Cl based on:

$$1.28\ C_3H_4N_2 + 1.28\ CH_3Cl \rightarrow C_4H_6N_2 \cdot HCl + 0.28\ C_3H_4N_2 + 0.28\ CH_3Cl$$

The specific enthalpies $\hat{H}$ for each chemical compound in the reaction were estimated according to eqn. (3) as follows:

$$\hat{H}_1/\hat{H}_3 = \Delta\hat{H}_f^o \text{ 1H-Imidazole (25 °C)} + \int_{25\ °C}^{100\ °C} Cp\ dT = 54.15\frac{kJ}{mol} + \left(0.0824\frac{kJ}{mol\ K} \text{ x } 75\ K\right) = 60.33\frac{kJ}{mol}$$

$$\hat{H}_2/\hat{H}_4 = \Delta\hat{H}_f^o \text{ Methyl chloride (25 °C)} + \int_{25\ °C}^{100\ °C} Cp\ dT = -102.4\frac{kJ}{mol} + \left(0.0812\frac{kJ}{mol\ K} \text{ x } 75\ K\right) = -96.31\frac{kJ}{mol}$$

$$\hat{H}_5 = \Delta\hat{H}_f^o \text{ [Hmim]Cl (25 °C)} + \int_{25\ °C}^{100\ °C} Cp\ dT = 206.2\frac{kJ}{mol} + \left(0.772\frac{kJ}{mol\ K} \text{ x } 75\ K\right) = 264.1\frac{kJ}{mol}$$

The enthalpy of the reaction was calculated using eqn. (S2) based on the specific enthalpy values $\hat{H}$ estimated for each chemical compound involved in the reaction of the synthesis of [Hmim]Cl as shown in Table S5. Hence:

$$\Delta H = \left[\left(1\text{ mol x } 264.1\frac{kJ}{mol}\right) + \left(0.28\text{ mol x } 60.33\frac{kJ}{mol}\right) + \left(0.28\text{ mol x } -96.31\frac{kJ}{mol}\right)\right] - \left[\left(1.28\text{ mol x } 60.33\frac{kJ}{mol}\right) + \left(1.28\text{ mol x } -96.31\frac{kJ}{mol}\right)\right]$$

$$= 300.08\ kJ$$

Thus, assuming that no work is carried and that kinetic and potential energy are zero (eqn. (S1)), the total amount of theoretical energy needed to heat the reactor is equal to 300.08 kJ or 0.30 MJ.

$$Q \approx \Delta H = 300.08\ kJ = 0.30\ MJ$$

The actual energy consumption was estimated by multiplying the above amount by a correction factor of 4.2 to convert the theoretical heat to the actual heat, assuming this is provided by natural gas. Therefore, the actual heat needed to heat the reactor is equal to 1.26 MJ.

Table S6 Input and output streams for the production of [Hmim]Cl

Chemical compound	n input (mol)	$\hat{H}$ input (kJ/mol)	n output (mol)	$\hat{H}$ output (kJ/mol)
1H-Imidazole	1.28	$\hat{H}1$	0.28	$\hat{H}3$
Methyl chloride	1.28	$\hat{H}2$	0.28	$\hat{H}4$
1-methylimidazole chloride	--	--	1	$\hat{H}5$

1H-Imidazole

Table S6 shows the input and output streams involved in the synthesis of 1H-Imidazole based on the following reaction:

$$1.5\ C_2H_2O_2 + 3\ NH_3 + 1.5\ CH_2O \rightarrow 1.28\ C_3H_4N_2 + 3.9\ H_2O + 0.23\ C_2H_2O_2 + 0.4\ NH_3 + 0.14\ CH_2O$$

The specific enthalpies $\hat{H}$ for the compounds involved in the synthesis of 1H-Imidazole were estimated according to eqn. (S3):

$$\hat{H}_1/\hat{H}_4 = \Delta\hat{H}_f^o \text{ Glyoxal (25 °C)} + \int_{25\ °C}^{75\ °C} Cp\ dT = -212\,\frac{kJ}{mol} + \left(0.0602\,\frac{kJ}{mol\ K} \times 50\ K\right) = -208.99\,\frac{kJ}{mol}$$

$$\hat{H}_2/\hat{H}_5 = \Delta\hat{H}_f^o \text{ Ammonia (25 °C)} + \int_{25\ °C}^{75\ °C} Cp\ dT = -45.92\,\frac{kJ}{mol} + \left(0.0356\,\frac{kJ}{mol\ K} \times 50\ K\right) = -44.14\,\frac{kJ}{mol}$$

$$\hat{H}_3/\hat{H}_6 = \Delta\hat{H}_f^o \text{ Formaldehyde (25 °C)} + \int_{25\ °C}^{75\ °C} Cp\ dT = -112.25\,\frac{kJ}{mol} + \left(0.0354\,\frac{kJ}{mol\ K} \times 50\ K\right) = -110.48\,\frac{kJ}{mol}$$

$$\hat{H}_7 = \Delta\hat{H}_f^o \text{ 1H-Imidazole (25 °C)} + \int_{25\ °C}^{75\ °C} Cp\ dT = 54.15\,\frac{kJ}{mol} + \left(0.0824\,\frac{kJ}{mol\ K} \times 50\ K\right) = 58.27\,\frac{kJ}{mol}$$

$$\hat{H}_8 = \Delta\hat{H}_f^o \text{ Water (25 °C)} + \int_{25\ °C}^{75\ °C} Cp\ dT = -285.83\,\frac{kJ}{mol} + \left(0.0754\,\frac{kJ}{mol\ K} \times 50\ K\right) = -282.06\,\frac{kJ}{mol}$$

The enthalpy of the reaction was calculated using eqn. (S2) based on the specific enthalpy values $\hat{H}$ estimated for each chemical compound involved in the reaction of the synthesis of 1H-imidazole as shown in Table S6. Hence:

$$\Delta H = \left[\left(1.28\ mol \times 58.27\,\frac{kJ}{mol}\right) + \left(3.9\ mol \times -282.06\,\frac{kJ}{mol}\right) + \left(0.23\ mol \times -208.99\,\frac{kJ}{mol}\right) + \left(0.4\ mol \times -44.14\,\frac{kJ}{mol}\right)\right.$$
$$\left. = \left(0.14\ mol \times -110.48\,\frac{kJ}{mol}\right)\right] - \left[\left(1.5\ mol \times -208.99\,\frac{kJ}{mol}\right) + \left(3\ mol \times -44.14\,\frac{kJ}{mol}\right) + \right.$$
$$\left.\left(1.5\ mol \times -110.48\,\frac{kJ}{mol}\right)\right] = -495\ kJ$$

A negative ΔH value indicates that an exothermic reaction is taking place and therefore heat needs to be removed through cooling. Therefore, the theoretical heat needed to be removed from the reactor is equal to:

$Q \approx \Delta H = -495\ kJ = -0.495\ MJ$

Using the correction factor 3.2, this heat is equivalent to 1.58 MJ of electricity needed to cool the reactor.

Table S7 Input and output streams for the production of [Hmim]Cl

Chemical compound	*n* input (mol)	$\hat{H}$ input (kJ/mol)	*n* output (mol)	$\hat{H}$ output (kJ/mol)
Glyoxal	1.5	$\hat{H}_1$	0.23	$\hat{H}_4$
Ammonia	3	$\hat{H}_2$	0.4	$\hat{H}_5$
Formaldehyde	1.5	$\hat{H}_3$	0.14	$\hat{H}_6$
1H-Imidazole	--	--	1.28	$\hat{H}_7$
Water	--	--	3.9	$\hat{H}_8$

Table S7 Conventional organic solvent production processes used from Ecoinvent [10] and their molecular weights.

Category	Solvent	MW (g/mol)	Process in Ecoinvent v3.8
Alcohols	Isopropanol	60	RER: isopropanol production
	Methanol	32	GLO: methanol production
	Propylene glycol	76	RER: propylene glycol production, liquid
Aliphatic hydrocarbons	Cyclohexane	84	RER: cyclohexane production
	Hexane[a]	86	GLO: market for hexane
Amine	Monoethanolamine[a]	61	GLO: market for monoethanolamine
Aromatic hydrocarbons	Toluene	92	RER: toluene production, liquid
	Xylene	106	RER: xylene production
Esters	Ethyl acetate	88	RER: ethyl acetate production
Ethers	Methyl tert-butyl ether	88	RER: methyl tert-butyl ether production
Halogenated solvents	Carbon tetrachloride	154	RER: carbon tetrachloride production
	Ethylene bromide	188	RER: ethylene bromide production
	Ethylene dichloride	99	RER: ethylene dichloride production
Ketones	Acetone	58	RER: acetone production, liquid
	Methyl ethyl ketone	72	RER: methyl ethyl ketone production
Sulfur containing	Dimethyl sulfate	126	RER: dimethyl sulfate production

[a] Production process not available in the database and a market was used instead.

Table S8. Linear coefficients of the GC model described by Equation (1) for each environmental property using both leave-one-out cross validation and bootstrap sampling. The root-mean-square error (RMSE) obtained by the linear GC model is also presented for each property.

	Linear coefficients β_i									
	Leave-one-out cross validation (*k*=18)					Bootstrap sampling (10,000 samples)				
Group	**GWP**	**HTP**	**FAETP**	**MAETP**	**TETP**	**GWP**	**HTP**	**FAETP**	**MAETP**	**TETP**
C_{im}	2.3306	10.0211	1.2088	22.1155	20.0724	2.3689	10.0491	1.2222	22.1689	20.3475
$C–(C)(N)(H)_2$	0.0393	0.029	0.0148	0.0301	0.3224	0.0735	0.0529	0.0281	0.0606	0.555
$C–(C)(H)_3$	0.1515	0.1133	0.0607	0.1084	1.1454	0.0822	0.0672	0.0351	0.071	0.6655
$C–(C)_2(H)_2$	0.0214	0.0281	0.0151	0.0279	0.2956	0.0214	0.028	0.0151	0.0276	0.2951
$C_b–(C)$	0.4031	0.2461	0.1283	0.2643	2.883	0.3582	0.2172	0.1129	0.2389	2.5642
$C_v–(C)$	0.1557	0.097	0.0557	0.1139	0.9976	0.0744	0.0433	0.0263	0.0449	0.4415
$C–(C_{im})(H)_3$	0.0064	0.004	0.0019	0.0036	0.041	-0.0109	-0.0174	-0.0062	-0.0959	-0.0921
Cl^-	-1.6415	-3.5362	-1.0486	-21.806	-16.6727	-1.6339	-3.5262	-1.0452	-21.7501	-16.6238
BF_4^-	-0.1441	-0.6921	0.0741	-12.9122	-3.016	-0.1471	-0.6947	0.0722	-12.911	-3.0314
$PF_6–$	1.7856	4.2283	0.9744	34.7182	19.6887	1.7811	4.2209	0.9729	34.6611	19.6551
RMSE	0.0392	0.2364	0.0142	0.0349	0.2603	0.0765	0.2939	0.0273	0.1802	0.5287

Sample calculations for predicting global warming impact of ionic liquids

Taking the ionic liquid 1-hexyl-3-methylimidazolium tetrafluoroborate $[C_6mim][BF_4]^-$ as an example (see chemical structure in Figure S1), the following global warming potential predictions can be obtained using the linear model proposed and presented in Equation S4 and the linear coefficients (β_i) reported in Table S8.

$$f = \sum_i n_i \beta_i \qquad (S4)$$

$$GWP = \sum_i n_i \beta_i^{GWP} \qquad (S5)$$

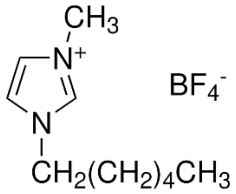

Figure S1 Chemical structure of 1-hexyl-3-methylimidazolium tetrafluoroborate

k-fold cross validation (LOOCV, *k*=18)

Substituting the corresponding terms in Equation S5 using the data presented in Table S8, we have the following:

$$\text{GWP} = [(1 \times 2.3306) + (1 \times 0.0393) + (4 \times 0.0214) + (1 \times 0.1515) + (1 \times (-0.1471))] = 2.4629$$

Bootstrap resampling

Substituting the corresponding terms in Equation S5 using the data presented in Table S8, we have the following:

$$\text{GWP} = [(1 \times 2.3689) + (1 \times 0.0735) + (4 \times 0.0214) + (1 \times 0.0822) + (1 \times (-0.1471))] = 2.4631$$

Table S9. Predicted global warming potential (GWP) of ionic liquid 1-hexyl-3-methylimidazolium tetrafluoroborate using the linear coefficients obtained via *k*-fold cross validation (LOOCV) and bootstrap resampling.

Chemical groups	n_i	β_i (LOOCV)	β_i (Bootstrap)	**LCA**[a]
C_{im}	1	2.3306	2.3689	-
$C\text{-}(C)(N)(H)_2$	1	0.0393	0.0735	-
$C\text{-}(C)_2(H)_2$	4	0.0214	0.0214	-
$C\text{-}(C)(H)_3$	1	0.1515	0.0822	-
BF_4^-	1	-0.1441	-0.1471	-
GW kg CO_2 eq./mol IL		2.4629	2.4631	2.4633
GW kg CO_2 eq./kg IL		9.6934	9.6942	9.6950

[a] Global warming potential estimated using the life cycle assessment (LCA) methodology in the present work.

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