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1-Carboxymethyl-3-octylimidazolium bromide

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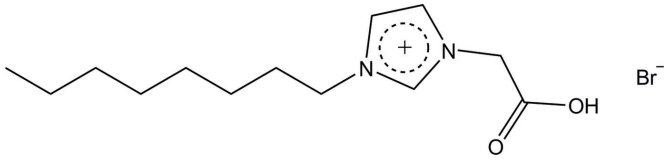
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.049; wR factor = 0.095; data-to-parameter ratio = 16.5.

In the title compound, $C_{13}H_{23}N_2O_2^+\cdot Br^-$, the octyl chain has an all-*trans* conformation. In the crystal, the cations are linked by C—H···O bonds into a zigzag chain along the *b* axis. The bromide anions further link the chains *via* C—H···Br interactions into a two-dimensional array parallel to the *ab* plane. An O—H···Br interaction is also observed.

Related literature

For related structures, see: Wei *et al.* (2009); Chen *et al.* (2009).



Experimental

Crystal data

$C_{13}H_{23}N_2O^{2+}\cdot Br^-$
M_r = 319.24
Monoclinic, $P2_1/c$
a = 7.6745 (2) Å
b = 4.6176 (1) Å
c = 41.8663 (9) Å
β = 92.167 (1)°
V = 1482.59 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.77 mm^{-1}
T = 100 K
0.21 × 0.19 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.594, T_{max} = 0.851
10905 measured reflections
2761 independent reflections
2678 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.095
S = 1.43
2761 reflections
167 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −2.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6B···Br1^{i}	0.99	2.89	3.772 (4)	148
C5—H5···Br1^{ii}	0.95	2.91	3.681 (4)	139
C4—H4···O2^{iii}	0.95	2.25	3.151 (5)	158
C3—H3···Br1^{i}	0.95	2.82	3.593 (4)	139
C2—H2B···Br1^{iv}	0.99	2.90	3.676 (4)	136
C2—H2A···O2^{v}	0.99	2.44	3.328 (5)	150
O1—H1···Br1	0.84 (2)	2.33 (2)	3.153 (3)	168 (4)

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $x, y+1, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2721).

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