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3-(Isobutyryloxy)propanaminium bromide

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.026
wR factor = 0.049
Data-to-parameter ratio = 24.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal packing in the title compound, $C_{10}H_{22}NO_2{}^{+}\cdot Br^{-}$, shows C—H···O and C—H···Br intermolecular hydrogen bonds, which give rise to stacking of the cations, as well as Br^{-} anions in rows along [010].

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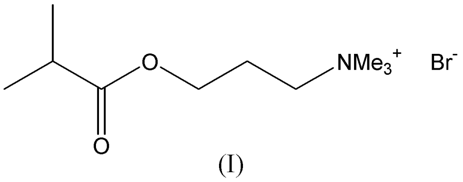
Comment

The title compound, (I), has been synthesized during a series of experiments to investigate the properties of surfactant esters of isobutyric acid and ω-trimethylammonium alcohols (Röder & Kramer, 2004). Accordingly, the alkyl chain length of the alcohol has been varied systematically. The propyl ester is that with the shortest chain. The longest one (decyl ester) shows a lyotropic mesophase (Hiltrop, 1994).



(I)

The molecular structure of (I) (Fig. 1) exhibits a folded conformation, with an O2—C5—C6—C7 torsion angle of −53.3 (2)°. This structure is related to that of the acetoxy compound 3-acetoxypropyltrimethylammonium bromide (Craven & Hite, 1973). The C5/O2/C4/O1/C3 ester group is planar, with a maximum deviation from the mean plane of 0.012 (1) Å for atom O2. An intramolecular C5—H5*B*···O1 hydrogen bond stabilizes this conformation, with H···O 2.39 Å. In general, bond lengths and angles (Table 1) lie in expected ranges and need no further discussion.

The crystal packing of (I) (Fig. 2) shows various intermolecular hydrogen bonds, with molecules stacked in rows along [010], and NMe_3 groups head-to-head and oriented in

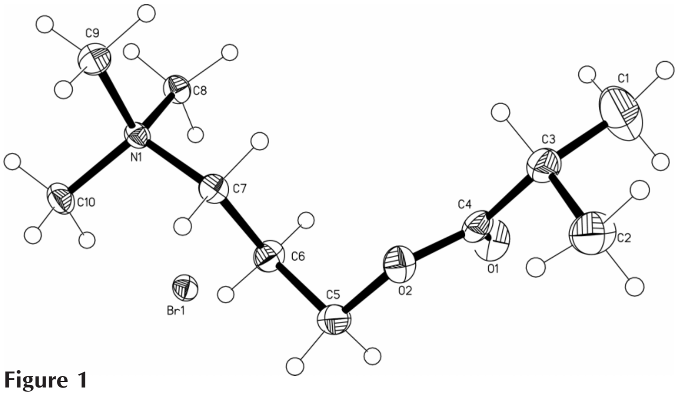


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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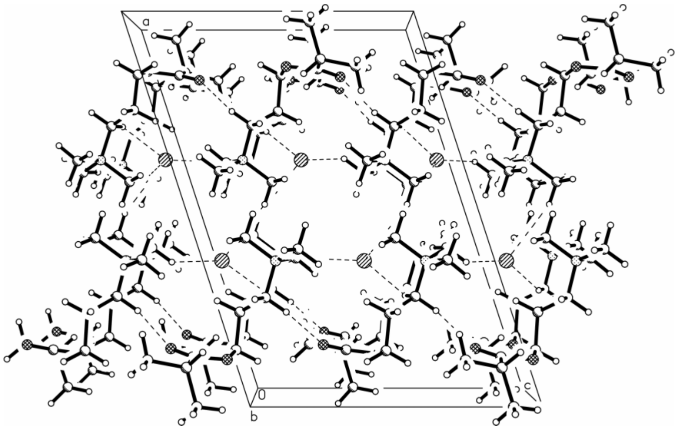

Figure 2
The crystal packing of (I), viewed along [010], with the intermolecular hydrogen-bonding pattern indicated by dashed lines.

the [100] direction. Prominent interactions are C7—H7*A*$\cdots$O1(x, $\frac{1}{2} - y$, $z + \frac{1}{2}$), with H$\cdots$O 2.32 Å and C—H$\cdots$O 145°, and four H$\cdots$Br contacts, C8—H8*C*$\cdots$Br(x, $y - 1$, z) (2.73 Å), C8—H8*A*$\cdots$Br($1 - x$, $y - \frac{1}{2}$, $\frac{3}{2} - z$) (2.83 Å), C7—H7*B*$\cdots$Br(x, $y - 1$, z) (2.84 Å) and C9—H9*C*$\cdots$Br(x, $\frac{1}{2} - y$, $z + \frac{1}{2}$) (2.89 Å). All H-atom positions were normalized to C—H = 1.08 Å.

Experimental

The synthesis of (I) was performed according to the method of Röder & Kramer (2004). After dissolving the compound in acetonitrile and allowing the solvent to evaporate slowly, fine prismatic crystals were obtained.

Crystal data

$C_{10}H_{22}NO_2^{+}\cdot Br^{-}$
$M_r = 268.20$
Monoclinic, $P2_1/c$
$a = 16.7315\ (14)$ Å
$b = 7.0370\ (6)$ Å
$c = 11.708\ (1)$ Å
$\beta = 107.979\ (2)°$
$V = 1311.18\ (19)$ Å^3
$Z = 4$
$D_x = 1.359$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3012 reflections
$\theta = 2.6$–$27.8°$
$\mu = 3.12$ mm^{-1}
$T = 120\ (2)$ K
Prism, colourless
$0.30 \times 0.15 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.581$, $T_{\max} = 0.782$
12 047 measured reflections
3276 independent reflections
2321 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.046$
$\theta_{\max} = 28.3°$
$h = -22 \rightarrow 22$
$k = -9 \rightarrow 9$
$l = -15 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.049$
$S = 0.84$
3276 reflections
132 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0155P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.46$ e Å^{-3}
$\Delta\rho_{\min} = -0.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C4	1.198 (2)	C3—C4	1.514 (3)
O2—C4	1.346 (2)	C5—C6	1.506 (2)
O2—C5	1.448 (2)	C6—C7	1.518 (3)
N1—C7	1.508 (2)		
C4—O2—C5	116.38 (16)	C5—C6—C7	109.65 (16)
O2—C4—C3	110.52 (19)	N1—C7—C6	115.20 (14)
O2—C5—C6	111.91 (15)		

H atoms were located in difference Fourier maps and then placed in calculated positions, with C—H distances in the range 0.98–0.99 Å, and treated as riding on their attached C atoms, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C) and $1.5U_{\rm eq}$(C-methyl). All CH_3 groups were allowed to rotate but not to tip.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2002); program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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