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Propyl 2-(5-bromo-3-methylsulfinyl-1-benzofuran-2-yl)acetate

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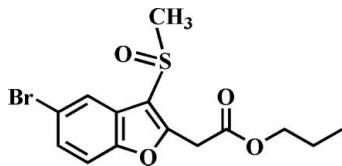
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.034; wR factor = 0.097; data-to-parameter ratio = 14.2.

In the title compound, $\text{C}_{14}\text{H}_{15}\text{BrO}_4\text{S}$, the S atom has a distorted trigonal-pyramidal coordination. The O atom and the methyl group of the methylsulfinyl substituent lie on opposite sides of the plane of the benzofuran fragment. The molecules form slightly slipped π -stacked inversion-symmetric dimers by intermolecular aromatic π - π interactions, with a centroid-to-centroid distance of 3.695 (4) Å between the benzene rings of neighbouring molecules. The crystal packing is further stabilized by intermolecular C—H... π interactions between the methylene H atoms of the propyl group towards the benzene and furan rings of neighbouring molecules, respectively. Additionally, the crystal structure exhibits weak intermolecular C—H...O hydrogen bonds.

Related literature

For the crystal structures of similar alkyl 2-(5-bromo-3-methylsulfinyl-1-benzofuran-2-yl)acetate derivatives, see: Choi *et al.* (2008a,b).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{15}\text{BrO}_4\text{S}$
 $M_r = 359.23$
 Triclinic, $P\bar{1}$
 $a = 8.4538$ (6) Å
 $b = 9.8823$ (7) Å
 $c = 10.3231$ (7) Å
 $\alpha = 72.358$ (1)°
 $\beta = 81.200$ (1)°
 $\gamma = 65.443$ (1)°
 $V = 747.16$ (9) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.90$ mm⁻¹
 $T = 298$ K
 $0.60 \times 0.50 \times 0.20$ mm

Data collection

Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1999)
 $T_{\min} = 0.187$, $T_{\max} = 0.556$
 3932 measured reflections
 2593 independent reflections
 2359 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.014$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.097$
 $S = 1.07$
 2593 reflections
 182 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.62$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.38$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
C11—H11B...Cg1 ⁱ	0.97	3.02	3.720 (3)	130
C12—H12B...Cg2 ⁱ	0.97	2.90	3.826 (3)	161
C3—H3...O4 ⁱⁱ	0.93	2.54	3.424 (3)	159
C5—H5...O3 ⁱⁱⁱ	0.93	2.58	3.430 (4)	152
C9—H9B...O4 ^{iv}	0.97	2.37	3.321 (3)	167

Symmetry codes: (i) $x, y - 1, z$; (ii) $-x + 1, -y + 1, -z + 2$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $-x, -y + 1, -z + 2$. Cg1 and Cg2 are the centroids of the C2–C7 benzene ring and the C1/C2/C7/O1/C8 furan ring, respectively.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and DIAMOND (Brandenburg, 1998); software used to prepare material for publication: SHELXL97.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2167).

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supporting information

Acta Cryst. (2009). E65, o520 [doi:10.1107/S160053680900453X]

Propyl 2-(5-bromo-3-methylsulfinyl-1-benzofuran-2-yl)acetate

Hong Dae Choi, Pil Ja Seo, Byeng Wha Son and Uk Lee

S1. Comment

As a part of our ongoing research on the synthesis and structure of alkyl 2-(5-bromo-3-methylsulfinyl-1-benzofuran-2-yl)acetate analogues, we have recently described the crystal structures of isopropyl 2-(5-bromo-3-methylsulfinyl-1-benzofuran-2-yl)acetate (Choi *et al.*, 2008a) and methyl 2-(5-bromo-3-methylsulfinyl-1-benzofuran-2-yl)acetate (Choi *et al.*, 2008b). Here we report the crystal structure of the title compound, propyl 2-(5-bromo-3-methylsulfinyl-1-benzofuran-2-yl)acetate (Fig. 1).

The benzofuran unit is essentially planar, with a mean deviation of 0.013 (2) Å from the least-squares plane defined by the nine constituent atoms. The molecular packing (Fig. 2) is stabilized by intermolecular π - π stacking interactions between the benzene rings of neighbouring molecules. Via this interaction the molecules form slightly slipped π -stacked inversion symmetric dimers, with a centroid-centroid distance $Cg1 \cdots Cg1^{iii}$ of 3.695 (4) Å between the benzene rings of neighbouring molecules. (Cg is the centroid of the C2-C7 benzene ring, symmetry code as in Fig. 2). The molecular packing is further stabilized by C-H \cdots π interactions; one between the hydrogen of the C11-methylene group and the benzene ring of the benzofuran unit, with a C11-H11B \cdots $Cg1^i$ separation of 3.02 Å, and a second between the hydrogen of the C12-methylene group and the furan ring of the benzofuran unit, with a C12-H12B \cdots $Cg2^i$ separation of 2.90 Å (Table 1 and Fig. 2; $Cg1$ and $Cg2$ are the centroids of the C2-C7 benzene ring and the C1/C2/C7/O1/C8 furan ring, respectively, symmetry code as in Fig. 2). In addition, three weak intermolecular C-H \cdots O hydrogen bonds in the structure were observed (Table 1 and Fig. 3); one between the hydrogen on benzene ring and the oxygen of the S=O unit (C3-H3 \cdots O4ⁱⁱ), a second between the hydrogen on benzene ring and the oxygen of the C=O unit (C5-H5 \cdots O3ⁱⁱⁱ), and a third between the hydrogen of the C9-methylene group and the S=O unit (C9-H9B \cdots O4^{iv}), respectively.

S2. Experimental

77% 3-chloroperoxybenzoic acid (179 mg, 0.8 mmol) was added in small portions to a stirred solution of propyl 2-(5-bromo-3-methylsulfonyl-1-benzofuran-2-yl)acetate (629 mg, 0.75 mmol) in dichloromethane (30 ml) at 273 K. After being stirred for 3 h at room temperature, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (hexane-ethyl acetate, 1:2 v/v) to afford the title compound as a colorless solid [yield 81%, m.p. 413-413.5 K; R_f = 0.55 (hexane-ethyl acetate, 1:2 v/v)]. Single crystals suitable for X-ray diffraction were prepared by evaporation of a solution of the title compound in benzene at room temperature. Spectroscopic analysis: ¹H NMR (CDCl₃, 400 MHz) δ 0.94 (t, J = 7.32 Hz, 3H), 1.63-1.72 (m, 2H), 3.07 (s, 3H), 4.05 (s, 2H), 4.11 (t, J = 6.96 Hz, 2H), 7.40 (d, J = 8.76 Hz, 1H), 7.48 (dd, J = 8.76 Hz and J = 1.84 Hz, 1H), 8.09 (d, J = 1.84 Hz, 1H); EI-MS 360 [M+2], 358 [M⁺].

S3. Refinement

All H atoms were geometrically positioned and refined using a riding model, with C—H = 0.93 Å for the aryl, 0.97 Å for the methylene, and 0.96 Å for the methyl H atoms. $U_{iso}(H) = 1.2U_{eq}(C)$ for the aryl and methylene H atoms, and $1.5U_{eq}(C)$ for methyl H atoms.

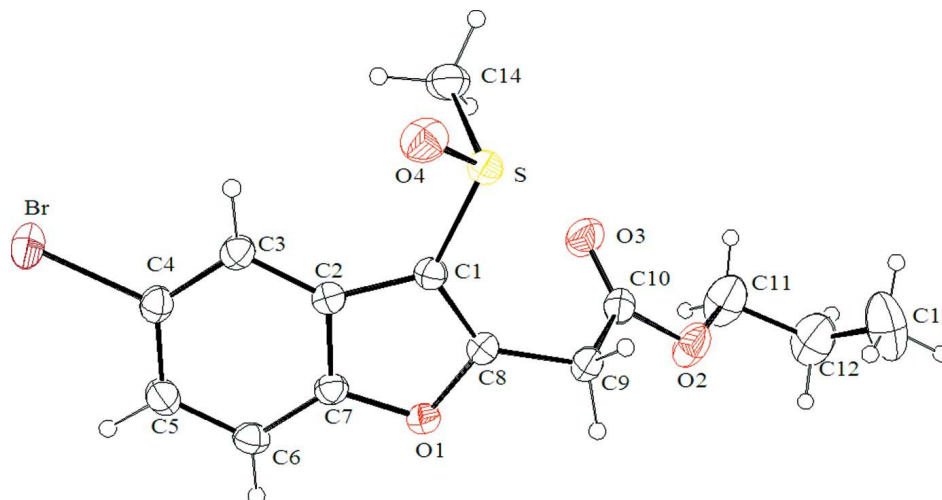


Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level.

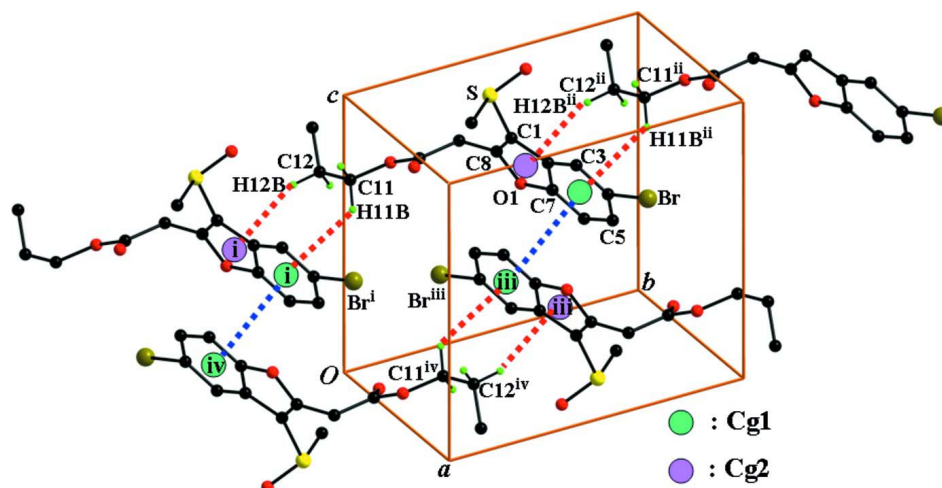


Figure 2

π — π and C—H... π interactions (dotted lines) in the title compound. Cg denotes the ring centroids. [Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+1, -y, -z+1$.]

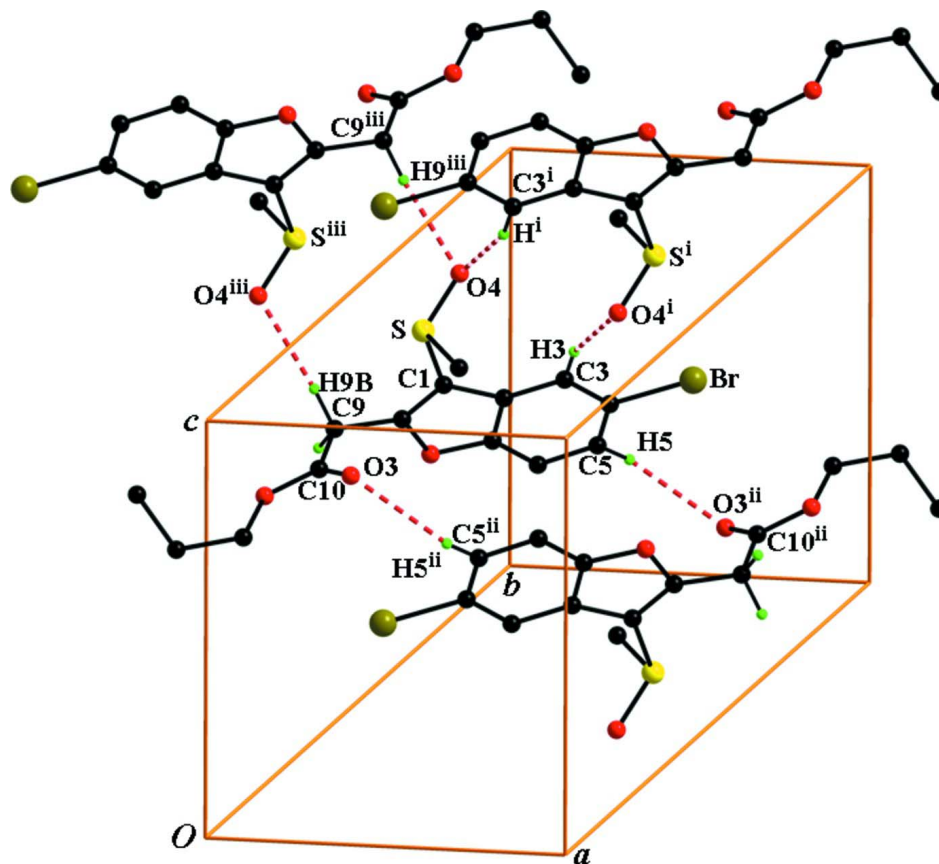


Figure 3

Intermolecular C—H...O hydrogen bonds (dotted lines) in the title compound. [Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x, -y+1, -z+2$.]

Propyl 2-(5-bromo-3-methylsulfinyl-1-benzofuran-2-yl)acetate

Crystal data

$C_{14}H_{15}BrO_4S$

$M_r = 359.23$

Triclinic, $P\bar{1}$

Hall symbol: $-p\ 1$

$a = 8.4538$ (6) Å

$b = 9.8823$ (7) Å

$c = 10.3231$ (7) Å

$\alpha = 72.358$ (1)°

$\beta = 81.200$ (1)°

$\gamma = 65.443$ (1)°

$V = 747.16$ (9) Å³

$Z = 2$

$F(000) = 364$

$D_x = 1.597$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2872 reflections

$\theta = 2.7$ – 28.0 °

$\mu = 2.90$ mm⁻¹

$T = 298$ K

Block, colourless

$0.60 \times 0.50 \times 0.20$ mm

Data collection

Bruker SMART CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.0 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1999)

$T_{\min} = 0.187$, $T_{\max} = 0.556$

3932 measured reflections

2593 independent reflections

2359 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.014$
 $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$
 $h = -9 \rightarrow 10$

$k = -10 \rightarrow 11$
 $l = -12 \rightarrow 10$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.097$
 $S = 1.07$
 2593 reflections
 182 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: difference Fourier map
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 0.3564P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.62 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.38 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br	0.68856 (4)	0.78591 (4)	0.61232 (4)	0.06138 (16)
S	0.26099 (9)	0.40306 (8)	0.96326 (6)	0.04277 (19)
O1	0.1656 (2)	0.5416 (2)	0.57292 (17)	0.0389 (4)
O2	0.0410 (3)	0.1435 (2)	0.7276 (3)	0.0651 (6)
O3	0.2856 (3)	0.1366 (3)	0.7909 (3)	0.0628 (6)
O4	0.2583 (3)	0.5257 (3)	1.0205 (2)	0.0565 (5)
C1	0.2557 (3)	0.4773 (3)	0.7850 (2)	0.0355 (5)
C2	0.3457 (3)	0.5694 (3)	0.6968 (2)	0.0345 (5)
C3	0.4701 (3)	0.6215 (3)	0.7124 (3)	0.0390 (6)
H3	0.5166	0.5970	0.7965	0.047*
C4	0.5206 (3)	0.7106 (3)	0.5974 (3)	0.0411 (6)
C5	0.4525 (4)	0.7510 (3)	0.4691 (3)	0.0448 (6)
H5	0.4882	0.8144	0.3949	0.054*
C6	0.3327 (3)	0.6968 (3)	0.4533 (3)	0.0421 (6)
H6	0.2877	0.7199	0.3689	0.051*
C7	0.2826 (3)	0.6069 (3)	0.5677 (3)	0.0367 (5)
C8	0.1513 (3)	0.4645 (3)	0.7068 (3)	0.0368 (5)
C9	0.0363 (3)	0.3784 (3)	0.7351 (3)	0.0408 (6)
H9A	-0.0412	0.4178	0.6600	0.049*
H9B	-0.0347	0.3956	0.8164	0.049*
C10	0.1380 (4)	0.2072 (3)	0.7546 (3)	0.0448 (6)
C11	0.1221 (5)	-0.0227 (4)	0.7402 (6)	0.0860 (14)

H11A	0.1843	-0.0769	0.8242	0.103*
H11B	0.2040	-0.0434	0.6648	0.103*
C12	-0.0195 (6)	-0.0757 (5)	0.7394 (6)	0.0900 (14)
H12A	-0.0800	-0.0196	0.6548	0.108*
H12B	0.0329	-0.1842	0.7418	0.108*
C13	-0.1468 (9)	-0.0548 (7)	0.8527 (6)	0.122 (2)
H13A	-0.2019	0.0527	0.8501	0.147*
H13B	-0.0889	-0.1122	0.9372	0.147*
H13C	-0.2332	-0.0913	0.8452	0.147*
C14	0.4798 (4)	0.2618 (4)	0.9755 (3)	0.0575 (8)
H14A	0.5592	0.3128	0.9465	0.086*
H14B	0.4965	0.1959	0.9185	0.086*
H14C	0.5011	0.2010	1.0681	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0581 (2)	0.0617 (2)	0.0766 (3)	-0.03898 (17)	-0.00471 (16)	-0.01173 (17)
S	0.0443 (4)	0.0525 (4)	0.0332 (3)	-0.0238 (3)	-0.0022 (3)	-0.0064 (3)
O1	0.0385 (9)	0.0443 (10)	0.0356 (9)	-0.0182 (8)	-0.0059 (7)	-0.0078 (8)
O2	0.0436 (11)	0.0429 (11)	0.114 (2)	-0.0170 (9)	-0.0113 (12)	-0.0243 (12)
O3	0.0443 (12)	0.0509 (12)	0.0865 (16)	-0.0157 (10)	-0.0153 (11)	-0.0066 (11)
O4	0.0607 (13)	0.0705 (14)	0.0457 (11)	-0.0259 (11)	0.0001 (10)	-0.0262 (10)
C1	0.0360 (12)	0.0366 (12)	0.0339 (12)	-0.0145 (10)	-0.0016 (10)	-0.0087 (10)
C2	0.0341 (12)	0.0333 (12)	0.0356 (12)	-0.0117 (10)	-0.0021 (10)	-0.0102 (10)
C3	0.0394 (13)	0.0395 (13)	0.0412 (14)	-0.0160 (11)	-0.0047 (10)	-0.0123 (11)
C4	0.0376 (13)	0.0365 (13)	0.0513 (16)	-0.0157 (11)	-0.0002 (11)	-0.0137 (11)
C5	0.0430 (14)	0.0394 (14)	0.0465 (15)	-0.0165 (12)	0.0019 (12)	-0.0049 (12)
C6	0.0429 (14)	0.0438 (14)	0.0348 (13)	-0.0143 (12)	-0.0048 (11)	-0.0060 (11)
C7	0.0335 (12)	0.0342 (12)	0.0409 (14)	-0.0108 (10)	-0.0047 (10)	-0.0097 (10)
C8	0.0340 (12)	0.0382 (13)	0.0373 (13)	-0.0142 (10)	-0.0016 (10)	-0.0084 (10)
C9	0.0366 (13)	0.0446 (14)	0.0449 (14)	-0.0186 (11)	-0.0029 (11)	-0.0123 (11)
C10	0.0401 (14)	0.0463 (15)	0.0491 (15)	-0.0210 (12)	-0.0001 (12)	-0.0089 (12)
C11	0.055 (2)	0.0450 (19)	0.158 (4)	-0.0120 (16)	-0.004 (2)	-0.039 (2)
C12	0.075 (3)	0.047 (2)	0.151 (4)	-0.0233 (18)	-0.005 (3)	-0.032 (2)
C13	0.138 (5)	0.095 (4)	0.140 (5)	-0.073 (4)	0.050 (4)	-0.026 (3)
C14	0.0550 (18)	0.0543 (18)	0.0555 (18)	-0.0142 (15)	-0.0160 (14)	-0.0075 (14)

Geometric parameters (Å, °)

Br—C4	1.899 (3)	C6—C7	1.374 (4)
S—O4	1.492 (2)	C6—H6	0.9300
S—C1	1.763 (3)	C8—C9	1.486 (4)
S—C14	1.790 (3)	C9—C10	1.509 (4)
O1—C8	1.375 (3)	C9—H9A	0.9700
O1—C7	1.375 (3)	C9—H9B	0.9700
O2—C10	1.323 (4)	C11—C12	1.494 (6)
O2—C11	1.465 (4)	C11—H11A	0.9700

O3—C10	1.202 (4)	C11—H11B	0.9700
C1—C8	1.349 (4)	C12—C13	1.465 (7)
C1—C2	1.448 (4)	C12—H12A	0.9700
C2—C3	1.396 (4)	C12—H12B	0.9700
C2—C7	1.397 (3)	C13—H13A	0.9600
C3—C4	1.376 (4)	C13—H13B	0.9600
C3—H3	0.9300	C13—H13C	0.9600
C4—C5	1.402 (4)	C14—H14A	0.9600
C5—C6	1.377 (4)	C14—H14B	0.9600
C5—H5	0.9300	C14—H14C	0.9600
O4—S—C1	107.01 (13)	C10—C9—H9A	109.2
O4—S—C14	106.32 (14)	C8—C9—H9B	109.2
C1—S—C14	98.46 (14)	C10—C9—H9B	109.2
C8—O1—C7	106.53 (19)	H9A—C9—H9B	107.9
C10—O2—C11	117.2 (2)	O3—C10—O2	124.0 (3)
C8—C1—C2	107.4 (2)	O3—C10—C9	125.6 (3)
C8—C1—S	123.4 (2)	O2—C10—C9	110.4 (2)
C2—C1—S	129.00 (19)	O2—C11—C12	107.7 (3)
C3—C2—C7	119.3 (2)	O2—C11—H11A	110.2
C3—C2—C1	136.1 (2)	C12—C11—H11A	110.2
C7—C2—C1	104.6 (2)	O2—C11—H11B	110.2
C4—C3—C2	116.8 (2)	C12—C11—H11B	110.2
C4—C3—H3	121.6	H11A—C11—H11B	108.5
C2—C3—H3	121.6	C13—C12—C11	114.4 (5)
C3—C4—C5	123.3 (3)	C13—C12—H12A	108.7
C3—C4—Br	118.7 (2)	C11—C12—H12A	108.7
C5—C4—Br	117.9 (2)	C13—C12—H12B	108.7
C6—C5—C4	119.8 (3)	C11—C12—H12B	108.7
C6—C5—H5	120.1	H12A—C12—H12B	107.6
C4—C5—H5	120.1	C12—C13—H13A	109.5
C7—C6—C5	117.1 (2)	C12—C13—H13B	109.5
C7—C6—H6	121.5	H13A—C13—H13B	109.5
C5—C6—H6	121.5	C12—C13—H13C	109.5
O1—C7—C6	125.9 (2)	H13A—C13—H13C	109.5
O1—C7—C2	110.5 (2)	H13B—C13—H13C	109.5
C6—C7—C2	123.6 (2)	S—C14—H14A	109.5
C1—C8—O1	111.0 (2)	S—C14—H14B	109.5
C1—C8—C9	133.2 (2)	H14A—C14—H14B	109.5
O1—C8—C9	115.7 (2)	S—C14—H14C	109.5
C8—C9—C10	112.2 (2)	H14A—C14—H14C	109.5
C8—C9—H9A	109.2	H14B—C14—H14C	109.5
O4—S—C1—C8	-134.5 (2)	C3—C2—C7—O1	178.3 (2)
C14—S—C1—C8	115.5 (2)	C1—C2—C7—O1	-1.2 (3)
O4—S—C1—C2	40.5 (3)	C3—C2—C7—C6	-1.8 (4)
C14—S—C1—C2	-69.5 (3)	C1—C2—C7—C6	178.8 (2)
C8—C1—C2—C3	-178.6 (3)	C2—C1—C8—O1	0.0 (3)

S—C1—C2—C3	5.7 (4)	S—C1—C8—O1	175.96 (17)
C8—C1—C2—C7	0.7 (3)	C2—C1—C8—C9	175.7 (3)
S—C1—C2—C7	-174.95 (19)	S—C1—C8—C9	-8.3 (4)
C7—C2—C3—C4	1.3 (4)	C7—O1—C8—C1	-0.7 (3)
C1—C2—C3—C4	-179.5 (3)	C7—O1—C8—C9	-177.3 (2)
C2—C3—C4—C5	0.6 (4)	C1—C8—C9—C10	-73.6 (4)
C2—C3—C4—Br	179.65 (18)	O1—C8—C9—C10	102.0 (3)
C3—C4—C5—C6	-2.0 (4)	C11—O2—C10—O3	-1.5 (5)
Br—C4—C5—C6	178.9 (2)	C11—O2—C10—C9	179.2 (3)
C4—C5—C6—C7	1.5 (4)	C8—C9—C10—O3	24.7 (4)
C8—O1—C7—C6	-178.8 (2)	C8—C9—C10—O2	-156.0 (2)
C8—O1—C7—C2	1.2 (3)	C10—O2—C11—C12	166.2 (4)
C5—C6—C7—O1	-179.7 (2)	O2—C11—C12—C13	-62.0 (6)
C5—C6—C7—C2	0.3 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C11—H11 <i>B</i> ...C <i>g</i> 1 ⁱ	0.97	3.02	3.720 (3)	130
C12—H12 <i>B</i> ...C <i>g</i> 2 ⁱ	0.97	2.90	3.826 (3)	161
C3—H3...O4 ⁱⁱ	0.93	2.54	3.424 (3)	159
C5—H5...O3 ⁱⁱⁱ	0.93	2.58	3.430 (4)	152
C9—H9 <i>B</i> ...O4 ^{iv}	0.97	2.37	3.321 (3)	167

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