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5-Bromo-2,4,6-trimethyl-3-(3-methylphenylsulfinyl)-1-benzofuran

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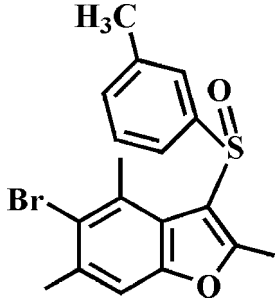
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.070; data-to-parameter ratio = 19.8.

In the title compound, $C_{18}H_{17}BrO_2S$, the dihedral angle between the mean plane of the benzofuran ring system and the benzene ring is 68.58 (4)°. In the crystal, molecules are linked *via* pairs of C—H···O hydrogen bonds into inversion dimers. These dimers are linked by C—H···O hydrogen bonds and π–π interactions between the benzene rings of neighbouring molecules [centroid–centroid distance = 3.783 (1) Å], forming a three-dimensional network. In addition, the stacked molecules exhibit inversion-related S···O contacts [3.153 (1) Å] involving the sulfinyl groups.

Related literature

For background information and the crystal structures of related compounds, see: Choi *et al.* (2008, 2011). For details of sulfinyl–sulfinyl interactions, see: Choi *et al.* (2013) and for a review of carbonyl–carbonyl interactions, see: Allen *et al.* (1998).



Experimental

Crystal data

$C_{18}H_{17}BrO_2S$
M_r = 377.29
Triclinic, $P\overline{1}$
a = 6.2336 (1) Å
b = 11.0353 (2) Å
c = 12.9149 (2) Å
α = 69.384 (1)°
β = 76.421 (1)°
γ = 76.799 (1)°
V = 797.84 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.71 mm^{-1}
T = 173 K
0.35 × 0.34 × 0.28 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.462, T_{max} = 0.746
14962 measured reflections
4023 independent reflections
3702 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.070
S = 1.06
4023 reflections
203 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1^{i}	0.95	2.50	3.4478 (19)	172
C11—H11A···O2^{ii}	0.98	2.36	3.244 (2)	150

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

Supporting information for this paper is available from the IUCr electronic archives (Reference: BX2455).

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supporting information

Acta Cryst. (2014). E**70**, o435 [doi:10.1107/S1600536814005352]

5-Bromo-2,4,6-trimethyl-3-(3-methylphenylsulfinyl)-1-benzofuran

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S1. Comment

As a part of our continuing study of 5-bromo-2,4,6-trimethyl-1-benzofuran derivatives containing phenylsulfinyl (Choi *et al.*, 2008) and 4-fluorophenylsulfinyl (Choi *et al.*, 2011) substituents in the 3-position, we report herein on the crystal structure of the title compound.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.027 (1) Å from the least-squares plane defined by the nine constituent atoms. The 3-methylphenyl ring is essentially planar, with a mean deviation of 0.011 (1) Å from the least-squares plane defined by the six constituent atoms. The dihedral angle formed by the benzofuran ring system and the 3-methylphenyl ring is 68.58 (4)°.

In the crystal structure (Fig. 2), molecules are linked via pairs of C–H···O hydrogen bonds into inversion dimers (Table 1). These dimers are further packed by C—H···O hydrogen bonds (Table 1) and $\pi\cdots\pi$ interactions between the benzene rings of neighbouring molecules, with a Cg1···Cg1^{iv} distance of 3.783 (1) Å and an interplanar distance of 3.402 (1) Å resulting in a slippage of 1.655 (1) Å (Cg1 is the centroid of the C2–C7 benzene ring), forming a three-dimensional network. In addition, the crystal packing (Fig. 2) exhibits a sulfinyl–sulfinyl interaction (Choi *et al.*, 2013) interpreted as similar to a type II carbonyl–carbonyl interaction (Allen *et al.* 1998), with S1···O2^{iii} and O2^{iii}···S1 distance of 3.153 (1) Å.

S2. Experimental

3-Chloroperoxybenzoic acid (77%, 269 mg, 1.2 mmol) was added in small portions to a stirred solution of 5-bromo-2,4,6-trimethyl-3-(3-methylphenylsulfanyl)-1-benzofuran (397 mg, 1.1 mmol) in dichloromethane (35 mL) at 273 K. After being stirred at room temperature for 5h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated at reduced pressure. The residue was purified by column chromatography (hexane–ethyl acetate, 2:1 *v*/*v*) to afford the title compound as a colorless solid [yield 72%, m.p. 469–470 K; R_f = 0.52 (hexane–ethyl acetate, 2:1 *v*/*v*)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in ethyl acetate at room temperature.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aryl and 0.95 Å for methyl H atoms. U_{iso} (H) = 1.2U_{eq} (C) for aryl and 1.5U_{eq} (C) for methyl H atoms. The positions of methyl hydrogens were optimized using the *SHELXL*-97's command AFIX 137 (Sheldrick, 2008).

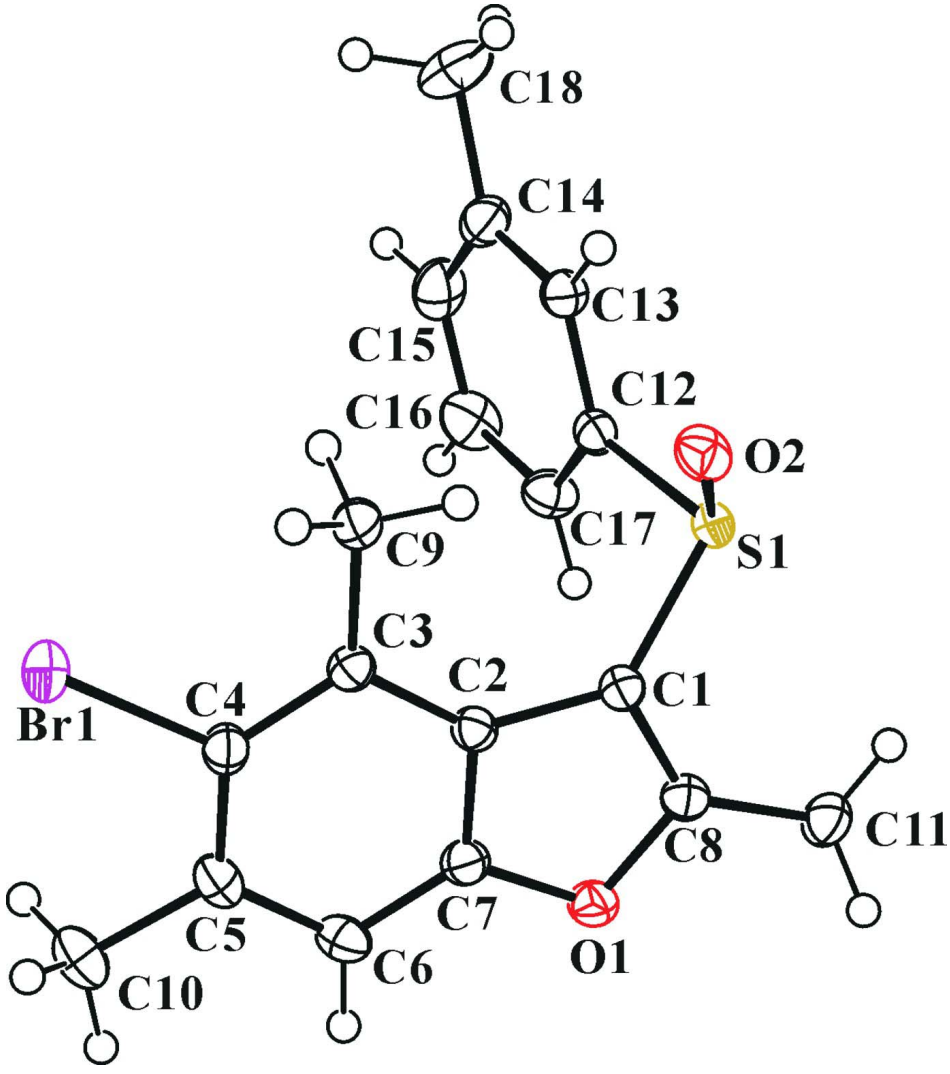

Figure 1

The molecular structure of the title molecule with the atom numbering scheme The displacement ellipsoids are drawn at the 50% probability level. The hydrogen atoms are presented as small spheres of arbitrary radius.

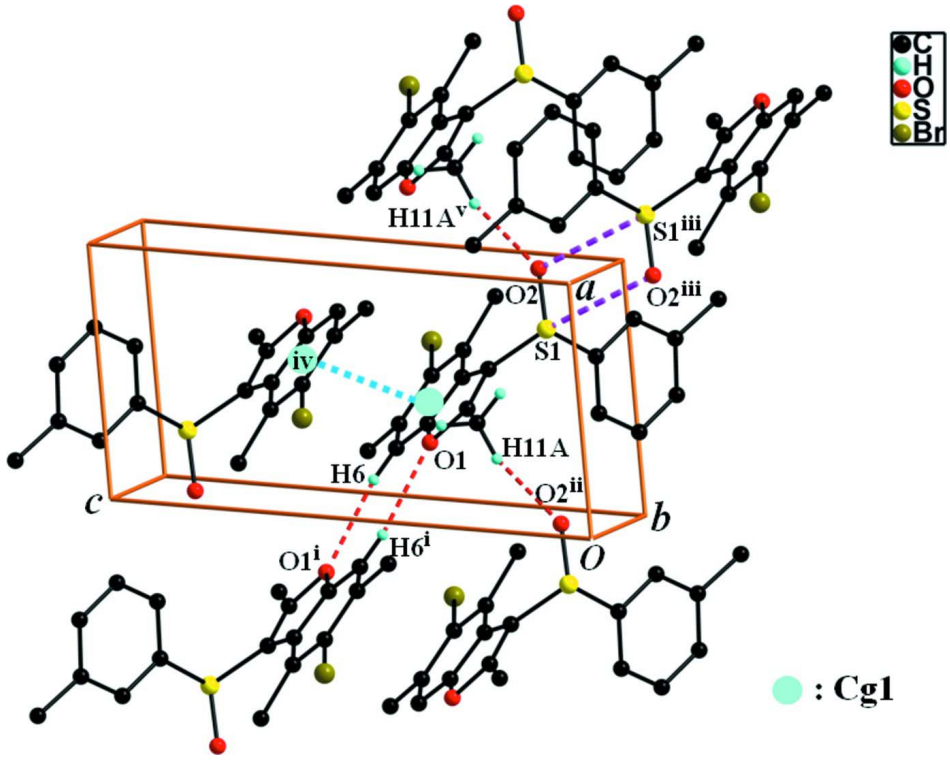

Figure 2

A view of the C—H···O, π···π and S···O interactions (dotted lines) in the crystal structure of the title compound. H atoms non-participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i) - x, - y + 1, - z + 1; (ii) x - 1, y, z; (iii) - x + 2, - y + 1, - z; (iv) - x + 1, -y + 1, - z + 1; (v) x + 1, y, z.]

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Crystal data

$C_{18}H_{17}BrO_2S$
M_r = 377.29
Triclinic, $P\overline{1}$
Hall symbol: -P 1
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c = 12.9149 (2) Å
α = 69.384 (1)°
β = 76.421 (1)°
γ = 76.799 (1)°
V = 797.84 (2) Å^3
Z = 2
F(000) = 384
D_x = 1.570 Mg m^{-3}
Melting point = 469–470 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8866 reflections
θ = 3.0–28.4°
μ = 2.71 mm^{-1}
T = 173 K
Block, colourless
0.35 × 0.34 × 0.28 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: rotating anode
Graphite multilayer monochromator
Detector resolution: 10.0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.462, T_{max} = 0.746
14962 measured reflections
4023 independent reflections
3702 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

θ_{max} = 28.4°, θ_{min} = 1.7°
h = −8→8
k = −14→14
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.070
S = 1.06
4023 reflections
203 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
$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 0.3061P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.62873 (3)	0.900826 (16)	0.403993 (14)	0.03223 (7)
S1	0.75692 (6)	0.51077 (3)	0.11568 (3)	0.01987 (9)
O1	0.27755 (19)	0.45708 (11)	0.37436 (9)	0.0241 (2)
O2	0.99335 (19)	0.51170 (11)	0.12084 (10)	0.0265 (2)
C1	0.5810 (3)	0.51004 (14)	0.24439 (12)	0.0196 (3)
C2	0.5305 (2)	0.59855 (14)	0.31119 (12)	0.0190 (3)
C3	0.6265 (3)	0.69926 (14)	0.31564 (12)	0.0195 (3)
C4	0.5100 (3)	0.76127 (15)	0.39418 (13)	0.0219 (3)
C5	0.3111 (3)	0.72874 (16)	0.46735 (13)	0.0244 (3)
C6	0.2268 (3)	0.62354 (17)	0.46533 (13)	0.0252 (3)
H6	0.0964	0.5954	0.5154	0.030*
C7	0.3399 (3)	0.56176 (15)	0.38791 (12)	0.0214 (3)
C8	0.4262 (3)	0.42809 (15)	0.28649 (12)	0.0221 (3)
C9	0.8457 (3)	0.73299 (16)	0.24263 (14)	0.0242 (3)
H9A	0.8171	0.8110	0.1782	0.036*
H9B	0.9253	0.6592	0.2159	0.036*
H9C	0.9372	0.7506	0.2863	0.036*
C10	0.1860 (3)	0.80420 (19)	0.54665 (16)	0.0341 (4)
H10A	0.0587	0.7619	0.5938	0.051*
H10B	0.1318	0.8943	0.5033	0.051*
H10C	0.2863	0.8054	0.5943	0.051*
C11	0.3854 (3)	0.31944 (16)	0.25548 (14)	0.0270 (3)
H11A	0.2470	0.3462	0.2240	0.041*

H11B	0.3713	0.2422	0.3224	0.041*
H11C	0.5108	0.2979	0.1995	0.041*
C12	0.6482 (3)	0.67448 (14)	0.03546 (12)	0.0198 (3)
C13	0.7999 (3)	0.75067 (15)	−0.04158 (12)	0.0225 (3)
H13	0.9557	0.7183	−0.0474	0.027*
C14	0.7230 (3)	0.87472 (16)	−0.11039 (14)	0.0275 (3)
C15	0.4952 (3)	0.92001 (17)	−0.09772 (15)	0.0329 (4)
H15	0.4411	1.0057	−0.1425	0.039*
C16	0.3449 (3)	0.84324 (19)	−0.02136 (15)	0.0337 (4)
H16	0.1893	0.8765	−0.0144	0.040*
C17	0.4195 (3)	0.71802 (17)	0.04509 (14)	0.0272 (3)
H17	0.3168	0.6635	0.0959	0.033*
C18	0.8835 (4)	0.9564 (2)	−0.19860 (17)	0.0443 (5)
H18A	0.8480	0.9733	−0.2729	0.066*
H18B	1.0366	0.9092	−0.1953	0.066*
H18C	0.8703	1.0399	−0.1850	0.066*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04364 (12)	0.02725 (10)	0.03175 (10)	−0.01115 (8)	−0.00252 (8)	−0.01557 (7)
S1	0.02068 (18)	0.01787 (17)	0.02010 (17)	−0.00149 (13)	−0.00020 (13)	−0.00790 (13)
O1	0.0248 (6)	0.0267 (6)	0.0223 (5)	−0.0103 (5)	0.0007 (4)	−0.0087 (4)
O2	0.0194 (5)	0.0287 (6)	0.0292 (6)	0.0009 (4)	−0.0019 (4)	−0.0109 (5)
C1	0.0212 (7)	0.0183 (6)	0.0185 (6)	−0.0026 (5)	−0.0023 (5)	−0.0058 (5)
C2	0.0199 (7)	0.0189 (7)	0.0174 (6)	−0.0019 (5)	−0.0029 (5)	−0.0054 (5)
C3	0.0205 (7)	0.0181 (6)	0.0187 (6)	−0.0028 (5)	−0.0033 (5)	−0.0047 (5)
C4	0.0260 (8)	0.0195 (7)	0.0216 (7)	−0.0031 (6)	−0.0054 (6)	−0.0076 (6)
C5	0.0247 (8)	0.0268 (8)	0.0220 (7)	0.0008 (6)	−0.0034 (6)	−0.0113 (6)
C6	0.0215 (7)	0.0319 (8)	0.0213 (7)	−0.0058 (6)	0.0009 (6)	−0.0093 (6)
C7	0.0226 (7)	0.0215 (7)	0.0199 (7)	−0.0058 (6)	−0.0030 (6)	−0.0054 (5)
C8	0.0253 (8)	0.0212 (7)	0.0190 (7)	−0.0041 (6)	−0.0039 (6)	−0.0052 (5)
C9	0.0231 (7)	0.0237 (7)	0.0269 (7)	−0.0071 (6)	0.0008 (6)	−0.0106 (6)
C10	0.0325 (9)	0.0390 (10)	0.0318 (9)	0.0002 (8)	0.0010 (7)	−0.0204 (8)
C11	0.0324 (9)	0.0236 (8)	0.0282 (8)	−0.0094 (7)	−0.0055 (7)	−0.0085 (6)
C12	0.0223 (7)	0.0191 (7)	0.0180 (6)	−0.0024 (6)	−0.0027 (5)	−0.0069 (5)
C13	0.0242 (8)	0.0235 (7)	0.0213 (7)	−0.0064 (6)	−0.0022 (6)	−0.0084 (6)
C14	0.0363 (9)	0.0243 (8)	0.0239 (7)	−0.0107 (7)	−0.0056 (7)	−0.0061 (6)
C15	0.0436 (11)	0.0230 (8)	0.0299 (8)	0.0011 (7)	−0.0140 (8)	−0.0047 (6)
C16	0.0266 (9)	0.0370 (10)	0.0324 (9)	0.0061 (7)	−0.0082 (7)	−0.0097 (7)
C17	0.0226 (8)	0.0304 (8)	0.0253 (8)	−0.0026 (6)	−0.0018 (6)	−0.0071 (6)
C18	0.0531 (13)	0.0348 (10)	0.0388 (10)	−0.0213 (9)	−0.0083 (9)	0.0051 (8)

Geometric parameters (Å, º)

Br1—C4	1.9073 (15)	C9—H9C	0.9800
S1—O2	1.4934 (12)	C10—H10A	0.9800
S1—C1	1.7619 (15)	C10—H10B	0.9800

S1—C12	1.8024 (15)	C10—H10C	0.9800
S1—O2^{i}	3.1527 (12)	C11—H11A	0.9800
O1—C8	1.3694 (19)	C11—H11B	0.9800
O1—C7	1.3770 (18)	C11—H11C	0.9800
C1—C8	1.361 (2)	C12—C13	1.387 (2)
C1—C2	1.457 (2)	C12—C17	1.387 (2)
C2—C7	1.393 (2)	C13—C14	1.392 (2)
C2—C3	1.401 (2)	C13—H13	0.9500
C3—C4	1.393 (2)	C14—C15	1.385 (3)
C3—C9	1.508 (2)	C14—C18	1.505 (2)
C4—C5	1.405 (2)	C15—C16	1.381 (3)
C5—C6	1.390 (2)	C15—H15	0.9500
C5—C10	1.510 (2)	C16—C17	1.386 (2)
C6—C7	1.375 (2)	C16—H16	0.9500
C6—H6	0.9500	C17—H17	0.9500
C8—C11	1.479 (2)	C18—H18A	0.9800
C9—H9A	0.9800	C18—H18B	0.9800
C9—H9B	0.9800	C18—H18C	0.9800

O2—S1—C1	111.08 (7)	C5—C10—H10A	109.5
O2—S1—C12	106.70 (7)	C5—C10—H10B	109.5
C1—S1—C12	96.91 (7)	H10A—C10—H10B	109.5
O2—S1—O2^{i}	78.25 (6)	C5—C10—H10C	109.5
C1—S1—O2^{i}	169.73 (6)	H10A—C10—H10C	109.5
C12—S1—O2^{i}	83.97 (5)	H10B—C10—H10C	109.5
C8—O1—C7	106.60 (12)	C8—C11—H11A	109.5
C8—C1—C2	107.12 (13)	C8—C11—H11B	109.5
C8—C1—S1	118.68 (12)	H11A—C11—H11B	109.5
C2—C1—S1	133.04 (11)	C8—C11—H11C	109.5
C7—C2—C3	119.45 (14)	H11A—C11—H11C	109.5
C7—C2—C1	104.27 (13)	H11B—C11—H11C	109.5
C3—C2—C1	136.25 (14)	C13—C12—C17	121.63 (14)
C4—C3—C2	115.39 (14)	C13—C12—S1	117.57 (12)
C4—C3—C9	123.20 (13)	C17—C12—S1	120.62 (12)
C2—C3—C9	121.37 (13)	C12—C13—C14	119.71 (15)
C3—C4—C5	125.00 (14)	C12—C13—H13	120.1
C3—C4—Br1	117.82 (11)	C14—C13—H13	120.1
C5—C4—Br1	117.18 (11)	C15—C14—C13	118.57 (16)
C6—C5—C4	118.23 (14)	C15—C14—C18	120.73 (16)
C6—C5—C10	119.23 (15)	C13—C14—C18	120.69 (17)
C4—C5—C10	122.54 (15)	C16—C15—C14	121.38 (16)
C7—C6—C5	117.29 (14)	C16—C15—H15	119.3
C7—C6—H6	121.4	C14—C15—H15	119.3
C5—C6—H6	121.4	C15—C16—C17	120.44 (17)
C6—C7—O1	124.56 (14)	C15—C16—H16	119.8
C6—C7—C2	124.45 (14)	C17—C16—H16	119.8
O1—C7—C2	110.98 (13)	C16—C17—C12	118.19 (16)
C1—C8—O1	110.99 (13)	C16—C17—H17	120.9

C1—C8—C11	133.49 (15)	C12—C17—H17	120.9
O1—C8—C11	115.50 (14)	C14—C18—H18A	109.5
C3—C9—H9A	109.5	C14—C18—H18B	109.5
C3—C9—H9B	109.5	H18A—C18—H18B	109.5
H9A—C9—H9B	109.5	C14—C18—H18C	109.5
C3—C9—H9C	109.5	H18A—C18—H18C	109.5
H9A—C9—H9C	109.5	H18B—C18—H18C	109.5
H9B—C9—H9C	109.5		

O2—S1—C1—C8	−136.06 (12)	C8—O1—C7—C2	−1.35 (16)
C12—S1—C1—C8	113.02 (13)	C3—C2—C7—C6	4.5 (2)
O2—S1—C1—C2	58.06 (17)	C1—C2—C7—C6	−177.07 (15)
C12—S1—C1—C2	−52.85 (16)	C3—C2—C7—O1	−176.74 (13)
C8—C1—C2—C7	−1.46 (16)	C1—C2—C7—O1	1.73 (16)
S1—C1—C2—C7	165.60 (13)	C2—C1—C8—O1	0.71 (17)
C8—C1—C2—C3	176.62 (17)	S1—C1—C8—O1	−168.54 (10)
S1—C1—C2—C3	−16.3 (3)	C2—C1—C8—C11	179.18 (16)
C7—C2—C3—C4	−4.3 (2)	S1—C1—C8—C11	9.9 (2)
C1—C2—C3—C4	177.88 (16)	C7—O1—C8—C1	0.35 (17)
C7—C2—C3—C9	173.53 (14)	C7—O1—C8—C11	−178.42 (13)
C1—C2—C3—C9	−4.3 (3)	O2—S1—C12—C13	25.77 (14)
C2—C3—C4—C5	0.9 (2)	C1—S1—C12—C13	140.27 (12)
C9—C3—C4—C5	−176.88 (15)	O2—S1—C12—C17	−158.95 (13)
C2—C3—C4—Br1	−179.31 (10)	C1—S1—C12—C17	−44.45 (14)
C9—C3—C4—Br1	2.9 (2)	C17—C12—C13—C14	0.8 (2)
C3—C4—C5—C6	2.7 (2)	S1—C12—C13—C14	176.07 (12)
Br1—C4—C5—C6	−177.13 (12)	C12—C13—C14—C15	1.6 (2)
C3—C4—C5—C10	−176.77 (15)	C12—C13—C14—C18	−176.88 (16)
Br1—C4—C5—C10	3.4 (2)	C13—C14—C15—C16	−2.1 (3)
C4—C5—C6—C7	−2.7 (2)	C18—C14—C15—C16	176.39 (18)
C10—C5—C6—C7	176.80 (15)	C14—C15—C16—C17	0.1 (3)
C5—C6—C7—O1	−179.40 (14)	C15—C16—C17—C12	2.3 (3)
C5—C6—C7—C2	−0.8 (2)	C13—C12—C17—C16	−2.8 (2)
C8—O1—C7—C6	177.44 (15)	S1—C12—C17—C16	−177.85 (13)

Symmetry code: (i) −*x*+2, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1^{ii}	0.95	2.50	3.4478 (19)	172
C11—H11*A*···O2^{iii}	0.98	2.36	3.244 (2)	150

Symmetry codes: (ii) −*x*, −*y*+1, −*z*+1; (iii) *x*−1, *y*, *z*.