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3-(4-Bromophenylsulfinyl)-2,4,6-trimethyl-1-benzofuran

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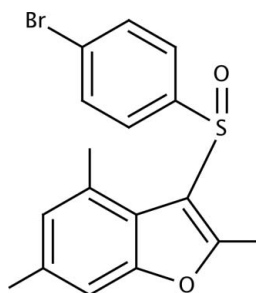
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.032; wR factor = 0.078; data-to-parameter ratio = 16.4.

In the title compound, $\text{C}_{17}\text{H}_{15}\text{BrO}_2\text{S}$, the 4-bromophenyl ring makes a dihedral angle of $87.12(6)^\circ$ with the mean plane of the benzofuran fragment. In the crystal, molecules are linked by weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For the pharmacological activity of benzofuran compounds, see: Aslam *et al.* (2009); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For the crystal structures of related compounds, see: Choi *et al.* (2010a,b).



Experimental

Crystal data

 $\text{C}_{17}\text{H}_{15}\text{BrO}_2\text{S}$ $M_r = 363.26$ Orthorhombic, Pna_21 $a = 12.0911(3)$ Å $b = 19.4713(3)$ Å $c = 6.4482(1)$ Å $V = 1518.10(5)$ Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 2.85$ mm⁻¹ $T = 173$ K $0.33 \times 0.29 \times 0.19$ mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.456$, $T_{\max} = 0.611$

8258 measured reflections
3190 independent reflections
2797 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.032$ $wR(F^2) = 0.078$ $S = 1.03$

3190 reflections

194 parameters

1 restraint

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.55$ e Å⁻³

Absolute structure: Flack (1983),

1131 Friedel pairs

Flack parameter: 0.014 (12)

Table 1

Hydrogen-bond geometry (Å, °).

C_g is the centroid of the C2–C7 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C11–H11C \cdots O2 ⁱ	0.98	2.59	3.343 (3)	134
C17–H17 \cdots O2 ⁱ	0.95	2.56	3.432 (3)	153
C4–H4 \cdots C _g ⁱⁱⁱ	0.95	2.89	3.724 (3)	147
C11–H11A \cdots C _g ⁱⁱⁱ	0.98	2.98	3.917 (3)	161

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

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 (Farrugia, 1997) and DIAMOND (Brandenburg, 1998); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2381).

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supporting information

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3-(4-Bromophenylsulfinyl)-2,4,6-trimethyl-1-benzofuran

Hong Dae Choi, Pil Ja Seo and Uk Lee

S1. Comment

Many compounds involving benzofuran skeleton have drawn much attention owing to their valuable biological properties such as antibacterial and antifungal, antitumor and antiviral, and antimicrobial activities (Aslam *et al.*, 2009, Galal *et al.*, 2009, Khan *et al.*, 2005). These benzofuran derivatives occur in a wide range of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing study of 2,4,6-trimethyl-1-benzofuran derivatives containing either 3-(4-fluorophenylsulfinyl) (Choi *et al.*, 2010a) or 3-(4-chlorophenylsulfinyl) (Choi *et al.*, 2010b) substituents, we report herein the crystal structure of the title compound.

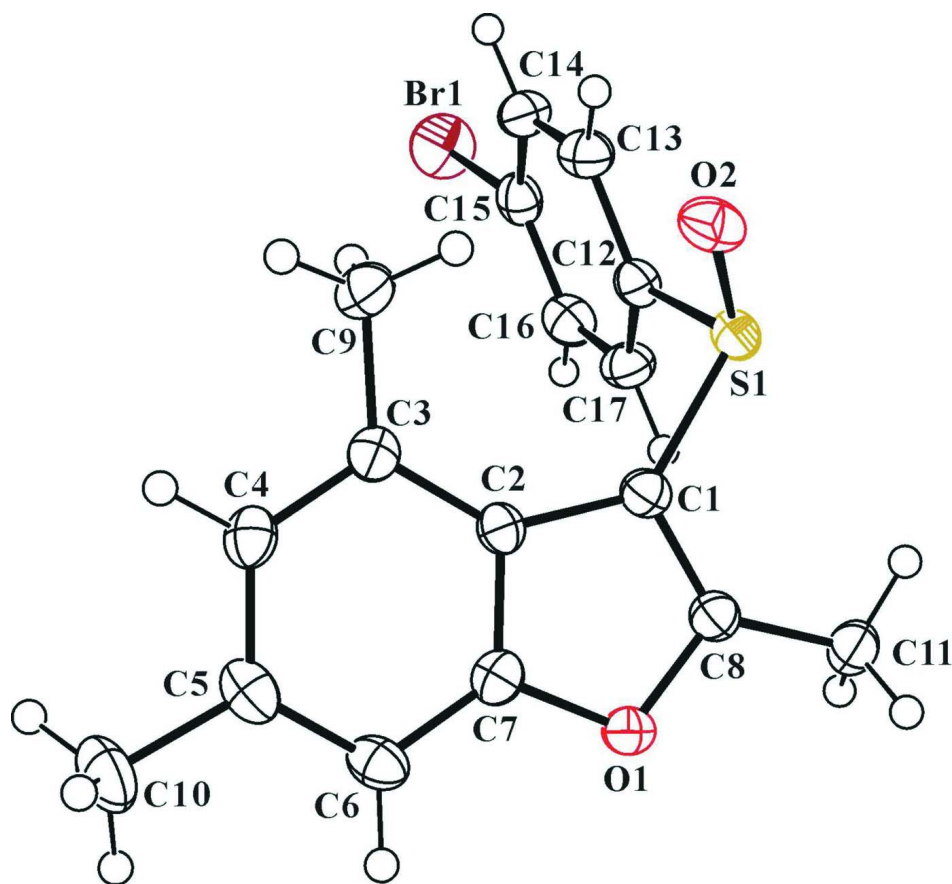
In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.009 (2) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle between the 4-bromophenyl ring and the mean plane of the benzofuran fragment is 87.12 (6)°. The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···O hydrogen bonds (see Table 1; first & second entry). The crystal packing (Fig. 3) is further stabilized by intermolecular C—H··· π interactions (see Table 1; third & fourth entry, Cg is the centroid of the C2–C7 benzene ring).

S2. Experimental

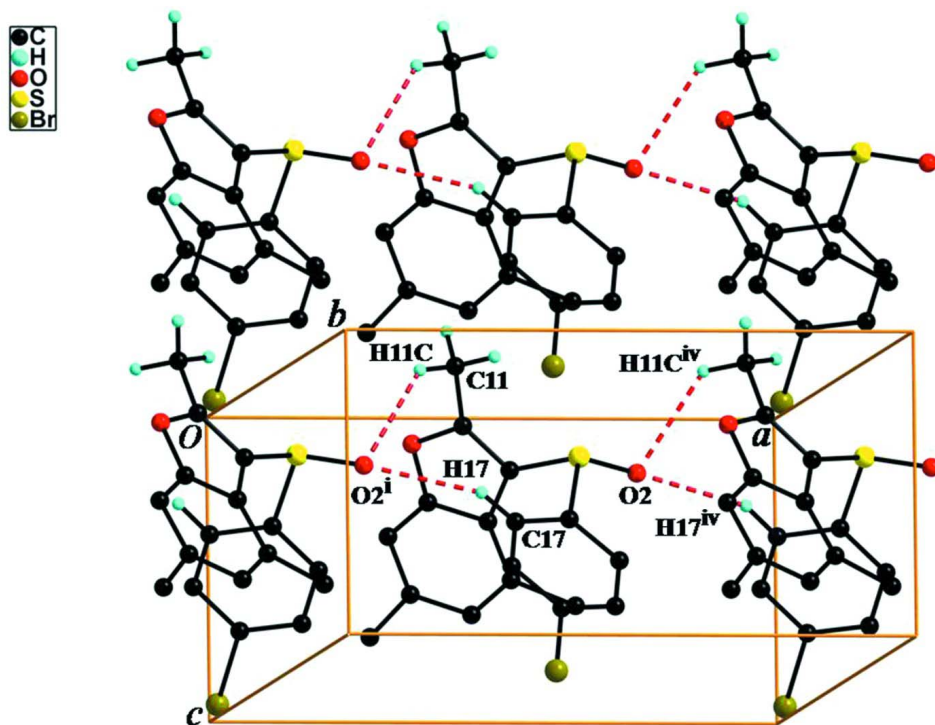
77% 3-chloroperoxybenzoic acid (224 mg, 1.0 mmol) was added in small portions to a stirred solution of 3-(4-bromophenylsulfinyl)-2,4,6-trimethyl-1-benzofuran (312 mg, 0.9 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 5h, the mixture was washed with saturated sodium 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 73%, m.p. 459–461 K; R_f = 0.54 (hexane–ethyl acetate, 4:1 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 0.98 Å for methyl H atoms. $U_{iso}(H) = 1.2U_{eq}(C)$ for aryl and $1.5U_{eq}(C)$ for methyl H atoms. The reported Flack parameter was obtained by the TWIN/BASF procedure in SHELXL (Sheldrick, 2008).

**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

**Figure 2**

A view of the C—H...O interactions (dotted lines) in the crystal structure of the title compound. H atoms not participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i) $x - 1/2, -y + 1/2, z$; (iv) $x + 1/2, -y + 1/2, z$.]

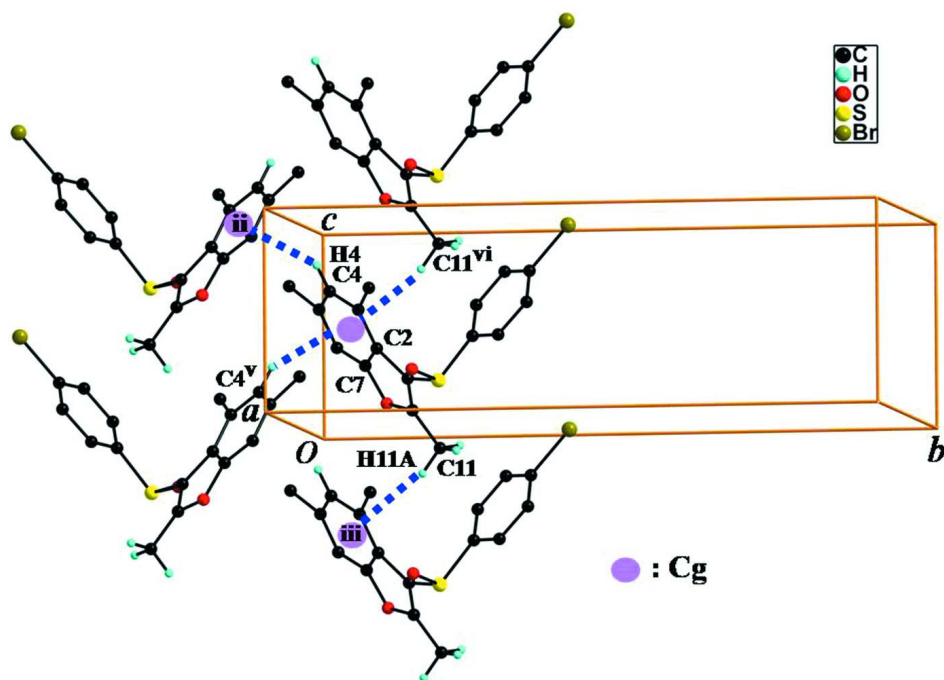


Figure 3

A view of the C—H... π interactions (dotted lines) in the crystal structure of the title compound. H atoms not participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (ii) $-x + 1, -y, z + 1/2$; (iii) $x, y, z - 1$; (v) $-x + 1, -y, z - 1/2$; (vi) $x, y, z + 1$.]

3-(4-Bromophenylsulfinyl)-2,4,6-trimethyl-1-benzofuran

Crystal data

$C_{17}H_{15}BrO_2S$

$M_r = 363.26$

Orthorhombic, $Pna2_1$

Hall symbol: $P\ 2c\ -2n$

$a = 12.0911\ (3)\ \text{\AA}$

$b = 19.4713\ (3)\ \text{\AA}$

$c = 6.4482\ (1)\ \text{\AA}$

$V = 1518.10\ (5)\ \text{\AA}^3$

$Z = 4$

$F(000) = 736$

$D_x = 1.589\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3220 reflections

$\theta = 2.7\text{--}27.0^\circ$

$\mu = 2.85\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Block, colourless

$0.33 \times 0.29 \times 0.19\ \text{mm}$

Data collection

Bruker SMART APEXII CCD
diffractometer

Radiation source: rotating anode

Multilayer monochromator

Detector resolution: $10.0\ \text{pixels mm}^{-1}$

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2009)

$T_{\min} = 0.456, T_{\max} = 0.611$

8258 measured reflections

3190 independent reflections

2797 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 28.3^\circ, \theta_{\min} = 2.0^\circ$

$h = -11 \rightarrow 16$

$k = -25 \rightarrow 21$

$l = -8 \rightarrow 7$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.078$
 $S = 1.03$
 3190 reflections
 194 parameters
 1 restraint
 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
 $w = 1/[\sigma^2(F_o^2) + (0.0362P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.55 \text{ e } \text{\AA}^{-3}$
 Absolute structure: Flack (1983), 1131 Friedel
 pairs
 Absolute structure parameter: 0.014 (12)

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.50103 (3)	0.448031 (17)	0.95844 (11)	0.04606 (11)
S1	0.59546 (5)	0.24377 (3)	0.19734 (12)	0.02620 (14)
O1	0.32864 (13)	0.13364 (8)	0.1240 (3)	0.0271 (4)
O2	0.70481 (13)	0.21095 (9)	0.2396 (3)	0.0337 (4)
C1	0.48796 (18)	0.18334 (13)	0.2236 (4)	0.0232 (5)
C2	0.4617 (2)	0.13067 (12)	0.3768 (4)	0.0218 (5)
C3	0.50764 (18)	0.10532 (15)	0.5613 (5)	0.0244 (6)
C4	0.4501 (2)	0.05337 (12)	0.6611 (4)	0.0280 (6)
H4	0.4799	0.0352	0.7859	0.034*
C5	0.3494 (2)	0.02600 (13)	0.5871 (5)	0.0300 (6)
C6	0.3051 (2)	0.05052 (12)	0.4044 (4)	0.0286 (6)
H6	0.2382	0.0327	0.3488	0.034*
C7	0.3631 (2)	0.10222 (12)	0.3065 (4)	0.0249 (5)
C8	0.4063 (2)	0.18286 (12)	0.0785 (4)	0.0244 (5)
C9	0.6138 (2)	0.13299 (14)	0.6532 (4)	0.0326 (6)
H9A	0.5976	0.1742	0.7350	0.049*
H9B	0.6653	0.1447	0.5413	0.049*
H9C	0.6472	0.0980	0.7428	0.049*
C10	0.2906 (2)	-0.02817 (14)	0.7122 (6)	0.0449 (7)
H10A	0.2119	-0.0282	0.6764	0.067*
H10B	0.2992	-0.0182	0.8603	0.067*
H10C	0.3225	-0.0733	0.6814	0.067*
C11	0.3837 (2)	0.22527 (13)	-0.1055 (4)	0.0290 (6)

H11A	0.3762	0.1956	-0.2275	0.043*
H11B	0.4449	0.2575	-0.1271	0.043*
H11C	0.3149	0.2510	-0.0846	0.043*
C12	0.5641 (2)	0.29687 (12)	0.4160 (4)	0.0246 (6)
C13	0.6479 (2)	0.31154 (13)	0.5558 (4)	0.0286 (6)
H13	0.7185	0.2908	0.5399	0.034*
C14	0.6288 (2)	0.35637 (12)	0.7187 (5)	0.0289 (6)
H14	0.6851	0.3657	0.8175	0.035*
C15	0.5266 (2)	0.38710 (13)	0.7346 (4)	0.0279 (6)
C16	0.4426 (2)	0.37384 (13)	0.5940 (5)	0.0306 (6)
H16	0.3728	0.3958	0.6080	0.037*
C17	0.4610 (2)	0.32882 (13)	0.4347 (5)	0.0299 (6)
H17	0.4041	0.3193	0.3373	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.05193 (19)	0.04310 (18)	0.04315 (19)	0.00241 (13)	0.00636 (14)	-0.01494 (17)
S1	0.0258 (3)	0.0285 (3)	0.0242 (3)	-0.0055 (2)	0.0024 (3)	0.0003 (3)
O1	0.0254 (9)	0.0279 (9)	0.0280 (10)	-0.0048 (8)	-0.0047 (8)	0.0031 (7)
O2	0.0234 (9)	0.0374 (10)	0.0401 (12)	-0.0016 (8)	0.0040 (8)	-0.0042 (8)
C1	0.0229 (12)	0.0234 (12)	0.0232 (14)	-0.0018 (9)	0.0018 (10)	-0.0029 (11)
C2	0.0216 (11)	0.0222 (12)	0.0216 (12)	0.0010 (10)	0.0030 (11)	-0.0001 (10)
C3	0.0229 (13)	0.0268 (14)	0.0234 (14)	0.0040 (9)	0.0016 (10)	0.0001 (11)
C4	0.0285 (13)	0.0277 (13)	0.0277 (16)	0.0068 (10)	-0.0001 (12)	0.0049 (10)
C5	0.0267 (13)	0.0230 (12)	0.0404 (16)	0.0036 (11)	0.0075 (12)	0.0047 (12)
C6	0.0218 (11)	0.0246 (12)	0.0395 (18)	0.0004 (9)	0.0007 (11)	0.0017 (11)
C7	0.0257 (12)	0.0244 (12)	0.0245 (14)	0.0041 (10)	-0.0008 (10)	0.0001 (10)
C8	0.0253 (12)	0.0246 (12)	0.0233 (13)	-0.0021 (10)	0.0010 (11)	-0.0020 (10)
C9	0.0289 (13)	0.0396 (14)	0.0293 (16)	0.0010 (12)	-0.0054 (12)	0.0023 (12)
C10	0.0357 (15)	0.0394 (15)	0.060 (2)	0.0003 (12)	0.0032 (17)	0.0258 (16)
C11	0.0296 (13)	0.0332 (13)	0.0241 (14)	0.0005 (11)	-0.0020 (11)	0.0012 (11)
C12	0.0255 (12)	0.0219 (12)	0.0264 (15)	-0.0037 (9)	-0.0003 (10)	0.0040 (10)
C13	0.0239 (13)	0.0287 (13)	0.0331 (15)	-0.0002 (11)	-0.0022 (11)	0.0003 (11)
C14	0.0261 (13)	0.0315 (13)	0.0293 (14)	-0.0018 (10)	-0.0050 (13)	0.0006 (12)
C15	0.0355 (13)	0.0219 (12)	0.0262 (15)	-0.0044 (10)	0.0030 (12)	-0.0001 (11)
C16	0.0258 (13)	0.0277 (14)	0.0382 (16)	0.0026 (11)	0.0022 (12)	0.0032 (12)
C17	0.0272 (12)	0.0281 (13)	0.0346 (15)	-0.0017 (11)	-0.0083 (14)	0.0042 (12)

Geometric parameters (Å, °)

Br1—C15	1.894 (3)	C9—H9A	0.9800
S1—O2	1.4935 (18)	C9—H9B	0.9800
S1—C1	1.761 (2)	C9—H9C	0.9800
S1—C12	1.789 (3)	C10—H10A	0.9800
O1—C8	1.373 (3)	C10—H10B	0.9800
O1—C7	1.390 (3)	C10—H10C	0.9800
C1—C8	1.360 (4)	C11—H11A	0.9800

C1—C2	1.459 (4)	C11—H11B	0.9800
C2—C7	1.390 (4)	C11—H11C	0.9800
C2—C3	1.403 (4)	C12—C13	1.386 (3)
C3—C4	1.386 (4)	C12—C17	1.398 (4)
C3—C9	1.513 (3)	C13—C14	1.385 (4)
C4—C5	1.412 (4)	C13—H13	0.9500
C4—H4	0.9500	C14—C15	1.377 (4)
C5—C6	1.380 (4)	C14—H14	0.9500
C5—C10	1.506 (4)	C15—C16	1.386 (4)
C6—C7	1.380 (3)	C16—C17	1.369 (4)
C6—H6	0.9500	C16—H16	0.9500
C8—C11	1.471 (4)	C17—H17	0.9500
O2—S1—C1	110.48 (11)	H9A—C9—H9C	109.5
O2—S1—C12	106.92 (11)	H9B—C9—H9C	109.5
C1—S1—C12	98.85 (12)	C5—C10—H10A	109.5
C8—O1—C7	106.43 (19)	C5—C10—H10B	109.5
C8—C1—C2	107.6 (2)	H10A—C10—H10B	109.5
C8—C1—S1	118.3 (2)	C5—C10—H10C	109.5
C2—C1—S1	134.1 (2)	H10A—C10—H10C	109.5
C7—C2—C3	118.4 (2)	H10B—C10—H10C	109.5
C7—C2—C1	104.2 (2)	C8—C11—H11A	109.5
C3—C2—C1	137.3 (2)	C8—C11—H11B	109.5
C4—C3—C2	116.8 (2)	H11A—C11—H11B	109.5
C4—C3—C9	120.2 (3)	C8—C11—H11C	109.5
C2—C3—C9	122.9 (2)	H11A—C11—H11C	109.5
C3—C4—C5	123.5 (2)	H11B—C11—H11C	109.5
C3—C4—H4	118.3	C13—C12—C17	120.3 (2)
C5—C4—H4	118.3	C13—C12—S1	118.47 (19)
C6—C5—C4	119.5 (2)	C17—C12—S1	120.92 (19)
C6—C5—C10	121.1 (3)	C14—C13—C12	120.1 (2)
C4—C5—C10	119.4 (3)	C14—C13—H13	119.9
C7—C6—C5	116.5 (2)	C12—C13—H13	119.9
C7—C6—H6	121.8	C15—C14—C13	118.7 (3)
C5—C6—H6	121.8	C15—C14—H14	120.7
C6—C7—O1	123.8 (2)	C13—C14—H14	120.7
C6—C7—C2	125.2 (2)	C14—C15—C16	121.9 (3)
O1—C7—C2	111.0 (2)	C14—C15—Br1	118.4 (2)
C1—C8—O1	110.8 (2)	C16—C15—Br1	119.7 (2)
C1—C8—C11	133.3 (2)	C17—C16—C15	119.4 (2)
O1—C8—C11	115.9 (2)	C17—C16—H16	120.3
C3—C9—H9A	109.5	C15—C16—H16	120.3
C3—C9—H9B	109.5	C16—C17—C12	119.6 (3)
H9A—C9—H9B	109.5	C16—C17—H17	120.2
C3—C9—H9C	109.5	C12—C17—H17	120.2
O2—S1—C1—C8	-136.6 (2)	C1—C2—C7—C6	-179.0 (2)
C12—S1—C1—C8	111.5 (2)	C3—C2—C7—O1	179.3 (2)

O2—S1—C1—C2	45.2 (3)	C1—C2—C7—O1	0.0 (3)
C12—S1—C1—C2	-66.7 (3)	C2—C1—C8—O1	-0.3 (3)
C8—C1—C2—C7	0.2 (3)	S1—C1—C8—O1	-179.02 (17)
S1—C1—C2—C7	178.6 (2)	C2—C1—C8—C11	176.7 (3)
C8—C1—C2—C3	-178.9 (3)	S1—C1—C8—C11	-2.0 (4)
S1—C1—C2—C3	-0.6 (5)	C7—O1—C8—C1	0.4 (3)
C7—C2—C3—C4	-0.3 (4)	C7—O1—C8—C11	-177.2 (2)
C1—C2—C3—C4	178.7 (3)	O2—S1—C12—C13	13.9 (2)
C7—C2—C3—C9	-179.3 (2)	C1—S1—C12—C13	128.6 (2)
C1—C2—C3—C9	-0.3 (5)	O2—S1—C12—C17	-172.8 (2)
C2—C3—C4—C5	-0.4 (4)	C1—S1—C12—C17	-58.1 (2)
C9—C3—C4—C5	178.6 (2)	C17—C12—C13—C14	2.0 (4)
C3—C4—C5—C6	1.1 (4)	S1—C12—C13—C14	175.40 (19)
C3—C4—C5—C10	-177.2 (3)	C12—C13—C14—C15	-1.8 (4)
C4—C5—C6—C7	-1.1 (4)	C13—C14—C15—C16	0.7 (4)
C10—C5—C6—C7	177.2 (2)	C13—C14—C15—Br1	179.7 (2)
C5—C6—C7—O1	-178.5 (2)	C14—C15—C16—C17	0.2 (4)
C5—C6—C7—C2	0.4 (4)	Br1—C15—C16—C17	-178.9 (2)
C8—O1—C7—C6	178.8 (2)	C15—C16—C17—C12	0.0 (4)
C8—O1—C7—C2	-0.2 (3)	C13—C12—C17—C16	-1.1 (4)
C3—C2—C7—C6	0.3 (4)	S1—C12—C17—C16	-174.3 (2)

Hydrogen-bond geometry (\AA , $^\circ$)

Cg is the centroid of the C2–C7 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C11—H11C \cdots O2 ⁱ	0.98	2.59	3.343 (3)	134
C17—H17 \cdots O2 ⁱ	0.95	2.56	3.432 (3)	153
C4—H4 \cdots Cg ⁱⁱ	0.95	2.89	3.724 (3)	147
C11—H11A \cdots Cg ⁱⁱⁱ	0.98	2.98	3.917 (3)	161

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