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3-(4-Bromophenylsulfonyl)-5-ethyl-2-methyl-1-benzofuran

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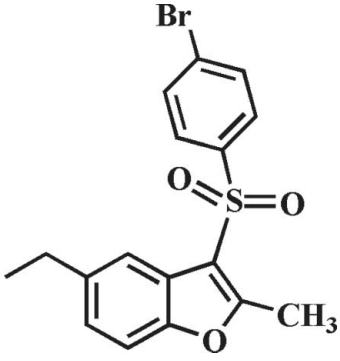
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.067; data-to-parameter ratio = 15.3.

In the title compound, $C_{17}H_{15}BrO_3S$, the 4-bromophenyl ring makes a dihedral angle of 76.58 (9)° with the mean plane [r.m.s. deviation = 0.006 (2) Å] of the benzofuran fragment. In the crystal, molecules are linked by weak C—H···O and C—H···π interactions.

Related literature

For the biological activity of benzofuran compounds, see: Aslam *et al.* (2009); Galal *et al.* (2009); Khan *et al.* (2005). For the crystal structures of related compounds, see: Choi *et al.* (2010, 2011).



Experimental

Crystal data

$C_{17}H_{15}BrO_3S$
M_r = 379.26
Tetragonal, $P4_3$
a = 10.2785 (3) Å
c = 15.2899 (6) Å
V = 1615.34 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.68 mm^{-1}
T = 173 K
0.31 × 0.17 × 0.15 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.450, T_{max} = 0.746
8518 measured reflections
3085 independent reflections
2558 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.067
S = 1.03
3085 reflections
201 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Absolute structure: Flack (1983), 1000 Friedel pairs
Flack parameter: 0.001 (7)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O3^{i}	0.95	2.53	3.238 (4)	131
C11—H11A···O3^{ii}	0.98	2.58	3.321 (4)	132
C14—H14···Cg^{iii}	0.95	2.70	3.495 (4)	142

Symmetry codes: (i) $-x, -y+1, z-\frac{1}{2}$; (ii) $-y+1, x, z-\frac{1}{4}$; (iii) $y, -x+1, z+\frac{1}{4}$.

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, 2012) 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: RN2111).

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supporting information

Acta Cryst. (2012). E**68**, o3487 [doi:10.1107/S1600536812048313]

3-(4-Bromophenylsulfonyl)-5-ethyl-2-methyl-1-benzofuran

Hong Dae Choi, Pil Ja Seo and Uk Lee

S1. Comment

Many compounds containing the benzofuran skeleton have attracted much interest owing to their 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). As a part of our ongoing study of 5-ethyl-2-methyl-1-benzofuran derivatives containing 4-fluorophenylsulfonyl (Choi *et al.*, 2010) or 3-fluorophenylsulfonyl (Choi *et al.*, 2011) substituents in the 3-position, we report herein the crystal structure of the title compound.

The title compound crystallizes as the non-centrosymmetric space group $P4_3$ in spite of having no asymmetric C atoms.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.006 (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 ring is 76.58 (9)°. In the crystal structure (Fig. 2), molecules are connected by weak C—H···O and C—H···π interactions (Table 1, Cg is the centroid of the C2–C7 benzene ring).

S2. Experimental

3-Chloroperoxybenzoic acid (77%, 448 mg, 2.0 mmol) was added in small portions to a stirred solution of 3-(4-bromophenylsulfanyl)-5-ethyl-2-methyl-1-benzofuran (312 mg, 0.9 mmol) in dichloromethane (50 mL) at 273 K. After being stirred at room temperature for 10h, 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 (benzene) to afford the title compound as a colorless solid [yield 68%, m.p. 404–405 K; R_f = 0.61 (benzene)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in diisopropyl ether 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, 0.99 Å for methylene and 0.98 Å for methyl H atoms, respectively. U_{iso}(H) = 1.2U_{eq}(C) for aryl, methylene, and 1.5U_{eq}(C) for methyl H atoms. The positions of methyl hydrogens were optimized rotationally.

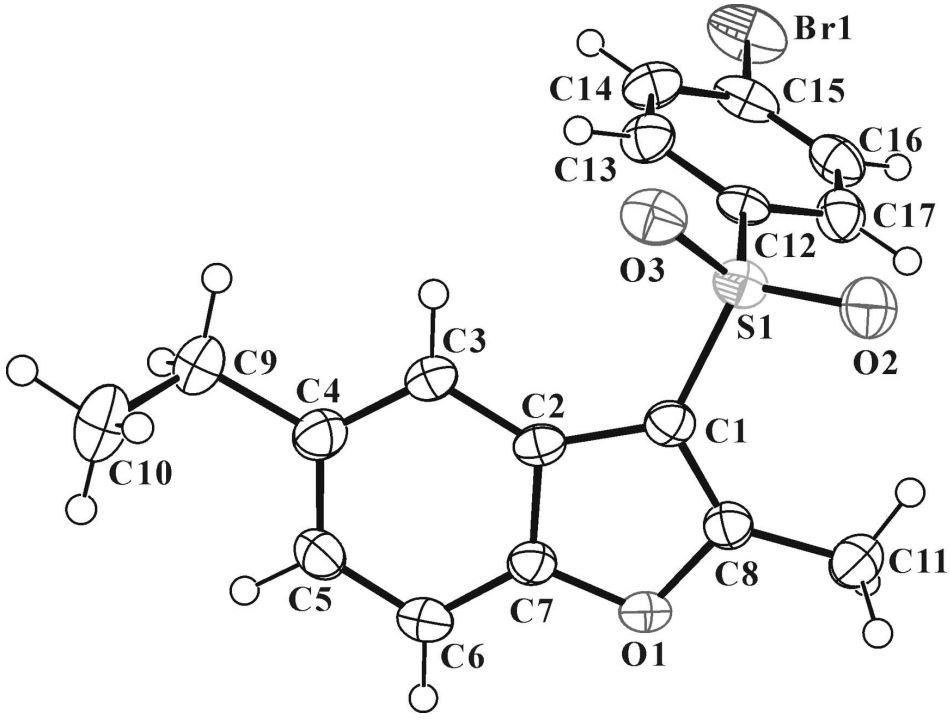

Figure 1

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

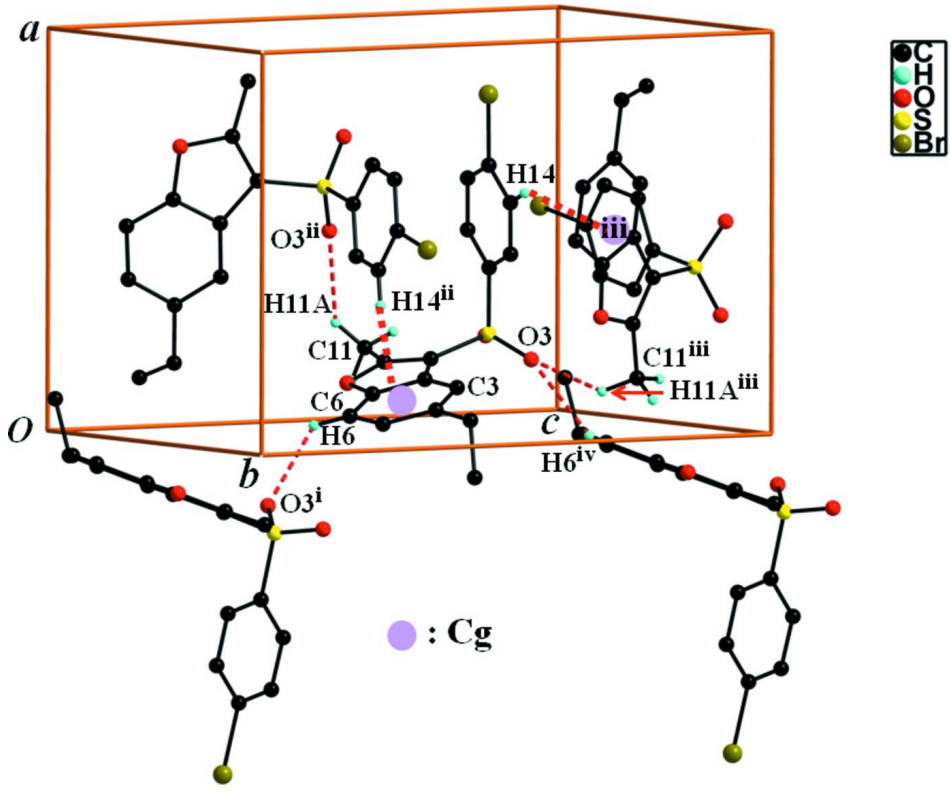

Figure 2

A view of the C—H···O and 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 code: (i) - x, - y + 1, z - 1/2 (ii) - y + 1, x, z - 1/4 (iii) y, - x + 1, z + 1/4 (iv) - x, - y + 1, z + 1/2

3-(4-Bromophenylsulfonyl)-5-ethyl-2-methyl-1-benzofuran

Crystal data

$C_{17}H_{15}BrO_3S$
M_r = 379.26
Tetragonal, $P4_3$
Hall symbol: P 4cw
a = 10.2785 (3) Å
c = 15.2899 (6) Å
V = 1615.34 (9) Å^3
Z = 4
F(000) = 768
D_x = 1.559 Mg m^{-3}
Melting point = 404–405 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2851 reflections
θ = 2.4–23.1°
μ = 2.68 mm^{-1}
T = 173 K
Block, colourless
0.31 × 0.17 × 0.15 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} = 0.450, T_{max} = 0.746
8518 measured reflections
3085 independent reflections
2558 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.3°, θ_{min} = 2.0°
h = −12→13
k = −13→12
l = −20→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.067$
$S = 1.03$
3085 reflections
201 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
$w = 1/[\sigma^2(F_o^2) + (0.0094P)^2 + 0.1451P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Absolute structure: Flack (1983), 1000 Friedel pairs
Absolute structure parameter: 0.001 (7)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.83341 (3)	0.52123 (5)	0.64403 (3)	0.06379 (15)
S1	0.22891 (7)	0.40370 (7)	0.69506 (5)	0.02917 (17)
O1	0.1117 (2)	0.2989 (2)	0.46167 (13)	0.0331 (5)
O2	0.2142 (2)	0.2825 (2)	0.73957 (15)	0.0401 (6)
O3	0.1697 (2)	0.5188 (2)	0.73023 (15)	0.0372 (5)
C12	0.3955 (3)	0.4357 (3)	0.68213 (18)	0.0248 (6)
C2	0.1292 (3)	0.4919 (3)	0.5329 (2)	0.0250 (6)
C17	0.4835 (3)	0.3333 (3)	0.6829 (2)	0.0357 (7)
H17	0.4546	0.2464	0.6912	0.043*
C13	0.4374 (3)	0.5626 (3)	0.6707 (2)	0.0346 (8)
H13	0.3763	0.6319	0.6705	0.042*
C16	0.6140 (3)	0.3604 (3)	0.6713 (2)	0.0394 (8)
H16	0.6757	0.2916	0.6712	0.047*
C15	0.6542 (3)	0.4857 (4)	0.66010 (19)	0.0390 (8)
C6	0.0458 (3)	0.4963 (3)	0.3844 (2)	0.0370 (7)
H6	0.0223	0.4525	0.3320	0.044*
C7	0.0933 (3)	0.4311 (3)	0.4558 (2)	0.0287 (7)
C5	0.0339 (3)	0.6299 (3)	0.3931 (3)	0.0382 (7)
H5	0.0008	0.6787	0.3452	0.046*
C3	0.1165 (3)	0.6262 (3)	0.5399 (2)	0.0299 (7)
H3	0.1403	0.6696	0.5923	0.036*
C8	0.1590 (3)	0.2747 (3)	0.5441 (2)	0.0295 (7)
C9	0.0514 (4)	0.8410 (3)	0.4760 (3)	0.0454 (9)

H9A	0.0846	0.8705	0.5335	0.054*
H9B	0.1046	0.8832	0.4301	0.054*
C14	0.5674 (3)	0.5881 (3)	0.6595 (2)	0.0392 (8)
H14	0.5971	0.6748	0.6515	0.047*
C4	0.0687 (3)	0.6956 (3)	0.4694 (2)	0.0359 (8)
C1	0.1709 (3)	0.3870 (3)	0.58850 (19)	0.0275 (7)
C11	0.1847 (3)	0.1373 (3)	0.5637 (2)	0.0399 (8)
H11A	0.2469	0.1025	0.5212	0.060*
H11B	0.1033	0.0880	0.5603	0.060*
H11C	0.2210	0.1297	0.6228	0.060*
C10	−0.0874 (4)	0.8851 (4)	0.4663 (3)	0.0598 (11)
H10A	−0.1202	0.8595	0.4086	0.090*
H10B	−0.0917	0.9799	0.4721	0.090*
H10C	−0.1409	0.8446	0.5119	0.090*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02640 (18)	0.1092 (4)	0.0558 (2)	−0.00760 (19)	0.00298 (19)	−0.0095 (3)
S1	0.0271 (4)	0.0358 (4)	0.0246 (3)	−0.0022 (3)	0.0028 (3)	−0.0006 (4)
O1	0.0342 (12)	0.0308 (12)	0.0344 (12)	−0.0039 (9)	−0.0097 (10)	−0.0053 (10)
O2	0.0447 (14)	0.0415 (14)	0.0340 (12)	−0.0079 (10)	0.0037 (11)	0.0077 (11)
O3	0.0330 (13)	0.0478 (14)	0.0308 (12)	0.0037 (10)	0.0048 (10)	−0.0083 (11)
C12	0.0189 (14)	0.0371 (17)	0.0183 (13)	−0.0009 (12)	0.0012 (12)	−0.0052 (13)
C2	0.0176 (14)	0.0285 (16)	0.0288 (16)	−0.0047 (12)	0.0025 (13)	−0.0043 (13)
C17	0.0399 (19)	0.0355 (18)	0.0316 (16)	0.0026 (13)	0.0022 (15)	0.0029 (15)
C13	0.0315 (17)	0.0337 (18)	0.0387 (19)	0.0036 (13)	0.0008 (14)	−0.0074 (14)
C16	0.0329 (18)	0.052 (2)	0.0330 (18)	0.0134 (15)	−0.0038 (14)	−0.0043 (16)
C15	0.0219 (15)	0.071 (3)	0.0243 (17)	−0.0017 (15)	0.0011 (14)	−0.0056 (17)
C6	0.0384 (18)	0.0387 (17)	0.0338 (17)	−0.0044 (14)	−0.0098 (16)	−0.0033 (16)
C7	0.0233 (15)	0.0279 (16)	0.0348 (17)	−0.0020 (12)	−0.0040 (13)	−0.0018 (14)
C5	0.0345 (18)	0.0388 (18)	0.0414 (17)	−0.0023 (14)	−0.0121 (17)	0.006 (2)
C3	0.0296 (17)	0.0273 (17)	0.0329 (17)	−0.0052 (13)	−0.0018 (14)	−0.0028 (14)
C8	0.0272 (17)	0.0302 (17)	0.0312 (17)	−0.0024 (13)	−0.0016 (14)	0.0012 (14)
C9	0.058 (2)	0.0264 (18)	0.052 (2)	−0.0003 (16)	−0.0081 (19)	0.0021 (16)
C14	0.0355 (18)	0.0398 (19)	0.042 (2)	−0.0093 (14)	0.0031 (16)	−0.0073 (16)
C4	0.0341 (18)	0.0313 (18)	0.0423 (19)	−0.0045 (13)	−0.0024 (15)	−0.0010 (15)
C1	0.0221 (16)	0.0302 (17)	0.0302 (16)	−0.0048 (12)	0.0000 (13)	0.0004 (14)
C11	0.043 (2)	0.0305 (18)	0.047 (2)	−0.0022 (15)	−0.0034 (17)	−0.0018 (16)
C10	0.072 (3)	0.034 (2)	0.074 (3)	0.0137 (18)	−0.004 (2)	0.000 (2)

Geometric parameters (Å, º)

Br1—C15	1.894 (3)	C6—C5	1.384 (4)
S1—O2	1.427 (2)	C6—H6	0.9500
S1—O3	1.435 (2)	C5—C4	1.395 (5)
S1—C1	1.743 (3)	C5—H5	0.9500
S1—C12	1.754 (3)	C3—C4	1.382 (4)

O1—C8	1.374 (4)	C3—H3	0.9500
O1—C7	1.376 (3)	C8—C1	1.345 (4)
C12—C13	1.385 (4)	C8—C11	1.467 (4)
C12—C17	1.388 (4)	C9—C10	1.505 (5)
C2—C7	1.384 (4)	C9—C4	1.509 (4)
C2—C3	1.391 (4)	C9—H9A	0.9900
C2—C1	1.438 (4)	C9—H9B	0.9900
C17—C16	1.381 (4)	C14—H14	0.9500
C17—H17	0.9500	C11—H11A	0.9800
C13—C14	1.372 (4)	C11—H11B	0.9800
C13—H13	0.9500	C11—H11C	0.9800
C16—C15	1.364 (5)	C10—H10A	0.9800
C16—H16	0.9500	C10—H10B	0.9800
C15—C14	1.381 (5)	C10—H10C	0.9800
C6—C7	1.371 (4)		

O2—S1—O3	119.73 (14)	C4—C3—C2	119.0 (3)
O2—S1—C1	108.87 (14)	C4—C3—H3	120.5
O3—S1—C1	106.63 (14)	C2—C3—H3	120.5
O2—S1—C12	108.70 (14)	C1—C8—O1	109.9 (3)
O3—S1—C12	107.56 (13)	C1—C8—C11	134.9 (3)
C1—S1—C12	104.29 (13)	O1—C8—C11	115.2 (3)
C8—O1—C7	106.7 (2)	C10—C9—C4	113.8 (3)
C13—C12—C17	120.8 (3)	C10—C9—H9A	108.8
C13—C12—S1	119.7 (2)	C4—C9—H9A	108.8
C17—C12—S1	119.6 (2)	C10—C9—H9B	108.8
C7—C2—C3	119.2 (3)	C4—C9—H9B	108.8
C7—C2—C1	104.2 (2)	H9A—C9—H9B	107.7
C3—C2—C1	136.6 (3)	C13—C14—C15	118.9 (3)
C16—C17—C12	118.7 (3)	C13—C14—H14	120.6
C16—C17—H17	120.7	C15—C14—H14	120.6
C12—C17—H17	120.7	C3—C4—C5	119.6 (3)
C14—C13—C12	120.0 (3)	C3—C4—C9	120.1 (3)
C14—C13—H13	120.0	C5—C4—C9	120.3 (3)
C12—C13—H13	120.0	C8—C1—C2	108.5 (3)
C15—C16—C17	120.1 (3)	C8—C1—S1	126.0 (2)
C15—C16—H16	120.0	C2—C1—S1	125.5 (2)
C17—C16—H16	120.0	C8—C11—H11A	109.5
C16—C15—C14	121.7 (3)	C8—C11—H11B	109.5
C16—C15—Br1	119.6 (3)	H11A—C11—H11B	109.5
C14—C15—Br1	118.7 (3)	C8—C11—H11C	109.5
C7—C6—C5	116.1 (3)	H11A—C11—H11C	109.5
C7—C6—H6	122.0	H11B—C11—H11C	109.5
C5—C6—H6	122.0	C9—C10—H10A	109.5
C6—C7—O1	125.7 (3)	C9—C10—H10B	109.5
C6—C7—C2	123.6 (3)	H10A—C10—H10B	109.5
O1—C7—C2	110.7 (3)	C9—C10—H10C	109.5
C6—C5—C4	122.5 (3)	H10A—C10—H10C	109.5

C6—C5—H5	118.7	H10B—C10—H10C	109.5
C4—C5—H5	118.7		
O2—S1—C12—C13	−156.8 (2)	C7—O1—C8—C11	179.7 (3)
O3—S1—C12—C13	−25.8 (3)	C12—C13—C14—C15	−0.1 (5)
C1—S1—C12—C13	87.2 (3)	C16—C15—C14—C13	0.1 (5)
O2—S1—C12—C17	23.7 (3)	Br1—C15—C14—C13	179.6 (2)
O3—S1—C12—C17	154.7 (2)	C2—C3—C4—C5	0.2 (5)
C1—S1—C12—C17	−92.3 (3)	C2—C3—C4—C9	178.8 (3)
C13—C12—C17—C16	−0.5 (4)	C6—C5—C4—C3	−0.3 (5)
S1—C12—C17—C16	179.1 (2)	C6—C5—C4—C9	−178.8 (3)
C17—C12—C13—C14	0.3 (4)	C10—C9—C4—C3	−117.6 (4)
S1—C12—C13—C14	−179.3 (3)	C10—C9—C4—C5	60.9 (5)
C12—C17—C16—C15	0.5 (5)	O1—C8—C1—C2	0.1 (3)
C17—C16—C15—C14	−0.3 (5)	C11—C8—C1—C2	180.0 (3)
C17—C16—C15—Br1	−179.8 (2)	O1—C8—C1—S1	−179.2 (2)
C5—C6—C7—O1	179.4 (3)	C11—C8—C1—S1	0.7 (5)
C5—C6—C7—C2	−0.4 (5)	C7—C2—C1—C8	0.2 (3)
C8—O1—C7—C6	−179.2 (3)	C3—C2—C1—C8	178.9 (3)
C8—O1—C7—C2	0.6 (3)	C7—C2—C1—S1	179.5 (2)
C3—C2—C7—C6	0.4 (5)	C3—C2—C1—S1	−1.8 (5)
C1—C2—C7—C6	179.3 (3)	O2—S1—C1—C8	−22.4 (3)
C3—C2—C7—O1	−179.4 (3)	O3—S1—C1—C8	−152.8 (3)
C1—C2—C7—O1	−0.5 (3)	C12—S1—C1—C8	93.5 (3)
C7—C6—C5—C4	0.4 (5)	O2—S1—C1—C2	158.4 (2)
C7—C2—C3—C4	−0.2 (4)	O3—S1—C1—C2	28.0 (3)
C1—C2—C3—C4	−178.8 (3)	C12—S1—C1—C2	−85.7 (3)
C7—O1—C8—C1	−0.4 (3)		

Hydrogen-bond geometry (Å, º)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O3^{i}	0.95	2.53	3.238 (4)	131
C11—H11*A*···O3^{ii}	0.98	2.58	3.321 (4)	132
C14—H14···*Cg*^{iii}	0.95	2.70	3.495 (4)	142

Symmetry codes: (i) −*x*, −*y*+1, *z*−1/2; (ii) −*y*+1, *x*, *z*−1/4; (iii) *y*, −*x*+1, *z*+1/4.