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3-Ethylsulfinyl-2-(4-iodophenyl)-5-methyl-1-benzofuran

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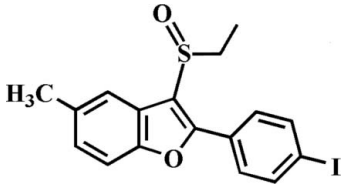
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.069; data-to-parameter ratio = 19.1.

In the title compound, $C_{17}H_{15}IO_2S$, the 4-iodophenyl ring makes a dihedral angle of 35.39 (8)° with the plane of the benzofuran fragment. In the crystal, molecules are linked by intermolecular C—H···O and C—H···π interactions, and an I···O contact [3.378 (2) Å]. The crystal structure also exhibits aromatic π–π interactions between the benzene rings of neighbouring molecules [centroid–centroid distance = 3.495 (3) Å].

Related literature

For the pharmacological activity of benzofuran compounds, see: Aslam *et al.* (2006); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For the structures of related 3-ethylsulfinyl-5-halo-2-(4-halophenyl)-1-benzofuran derivatives, see: Choi *et al.* (2010*a*,*b*,*c*). For a review of halogen bonding, see: Politzer *et al.* (2007).



Experimental

Crystal data

$C_{17}H_{15}IO_2S$
M_r = 410.25
Monoclinic, $P2_1/n$
a = 10.1034 (3) Å
b = 13.1942 (4) Å
c = 11.9933 (3) Å
β = 92.634 (1)°
V = 1597.09 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.14 mm^{-1}
T = 173 K
0.32 × 0.27 × 0.09 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.551, T_{max} = 0.834
15129 measured reflections
3667 independent reflections
3366 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.069
S = 1.07
3667 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

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
C16—H16B···O2^{i}	0.97	2.60	3.341 (3)	134
C11—H11···Cg^{ii}	0.93	2.61	3.378 (3)	141

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

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2357).

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supporting information

Acta Cryst. (2010). E**66**, o1985 [https://doi.org/10.1107/S1600536810026620]

3-Ethylsulfinyl-2-(4-iodophenyl)-5-methyl-1-benzofuran

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

S1. Comment

The benzofuran ring system show interesting pharmacological properties such as antifungal (Aslam *et al.*, 2006), antitumor and antiviral (Galal *et al.*, 2009), antimicrobial (Khan *et al.*, 2005) activities. These compounds widely occur in nature (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our continuing studies of the substituent effect on the solid state structures of 3-ethylsulfinyl-5-halo-2-(4-halophenyl)-1-benzofuran analogues (Choi *et al.*, 2010*a,b,c*), we report the crystal structure of the title compound (Fig. 1).

The benzofuran unit is essentially planar, with a mean deviation of 0.021 (2) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle formed by the benzofuran plane and the 4-iodophenyl ring is 35.39 (8)°. The crystal packing (Fig. 2) is stabilized by a weak intermolecular C—H···O hydrogen bond between the methylene H atom of the ethyl group and the oxygen of the S═O unit, with a C16—16B···O2^{i} (Table 1), and by an I···O halogen-bonding between the iodine and the oxygen of the S═O unit [I···O2^{iii} = 3.378 (2) Å; C12—I···O2^{iii} = 162.46 (7)°] (Politzer *et al.*, 2007). The molecular packing (Fig. 3) is further stabilized by an intermolecular C—H···π interaction between the 4-iodophenyl H atom and the benzene ring of a neighbouring molecule, with a C11—H11···Cg^{ii} (Table 1), and by an aromatic π–π interaction between the benzene rings of neighbouring molecules, with a Cg···Cg^{v} distance of 3.495 (3) Å (Cg is the centroid of the C2–C7 benzene ring).

S2. Experimental

77% 3-chloroperoxybenzoic acid (202 mg, 0.9 mmol) was added in small portions to a stirred solution of 3-ethyl-sulfanyl-2-(4-iodophenyl)-5-methyl-1-benzofurans (315 mg, 0.8 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 4h, 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, 1:2 v/v) to afford the title compound as a colorless solid [yield 79%, m.p. 431–432 K; R_f = 0.63 (hexane–ethyl acetate, 1:2 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in tetrahydrofuran at room temperature.

S3. Refinement

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

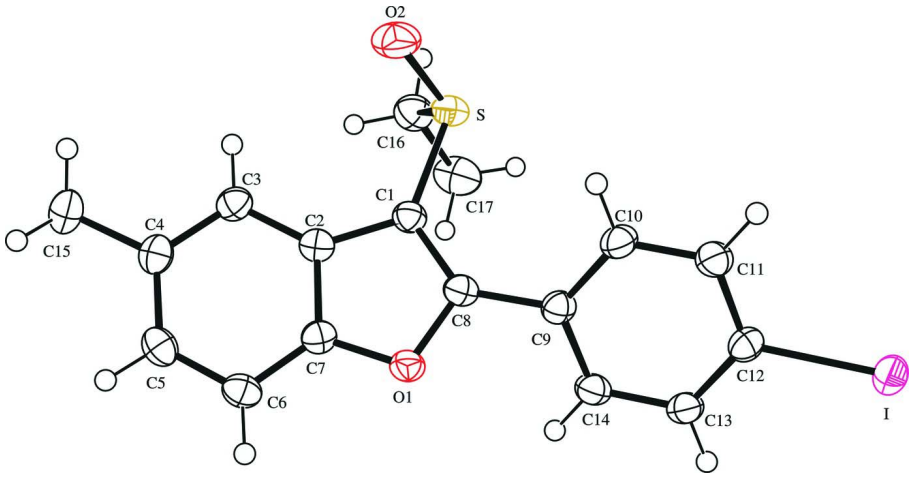

Figure 1

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 a small spheres of arbitrary radius.

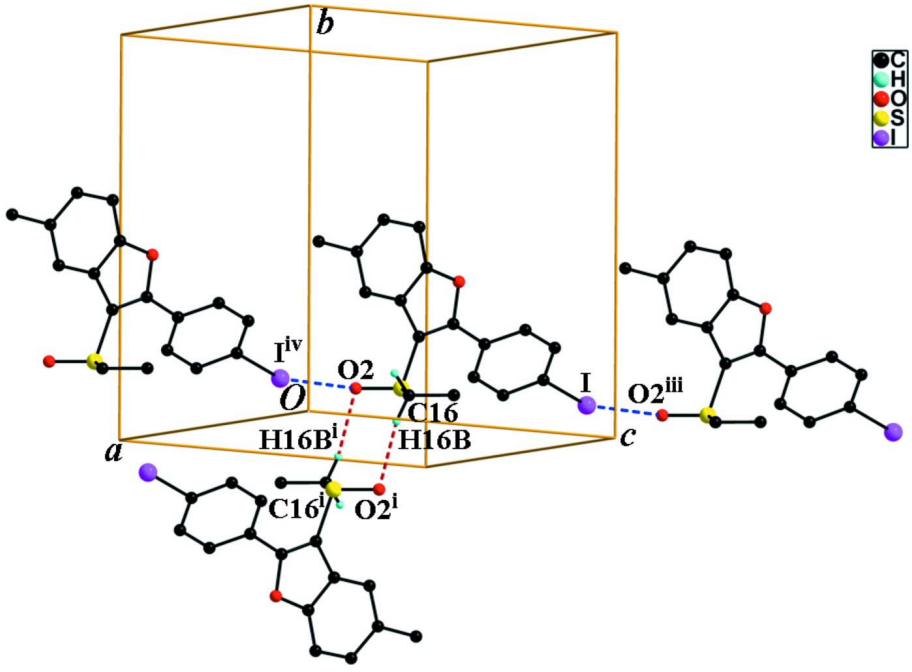

Figure 2

C–H···O and I···O interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) -*x* + 1, -*y*, -*z* + 1; (iii) *x*, *y*, *z* + 1; (iv) *x*, *y*, *z* -1 .]

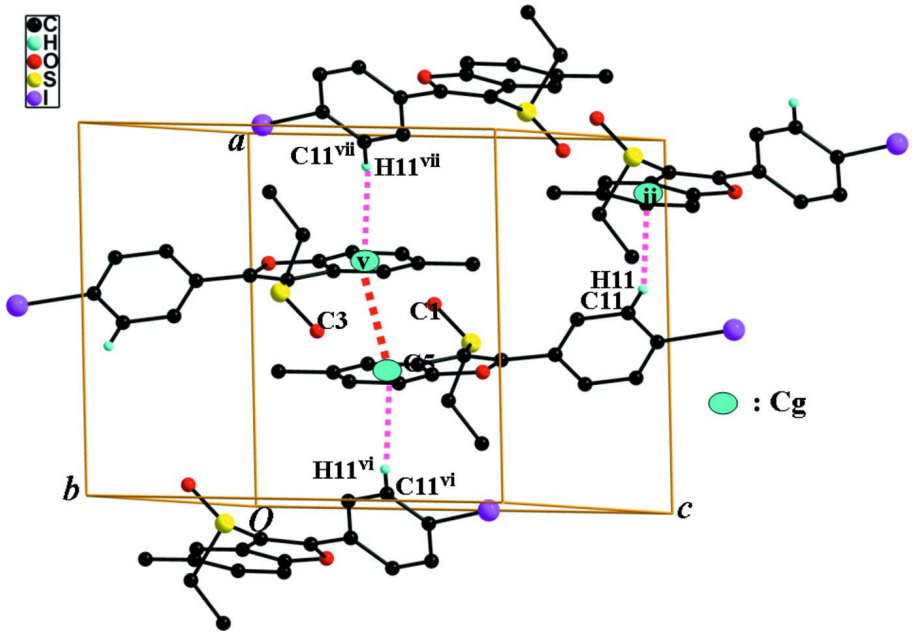

Figure 3

C–H···π, and π–π interactions (dotted lines) in the crystal structure of the title compound. Cg denotes the ring centroid. [Symmetry codes: (ii) x + 1/2, -y + 1/2, z + 1/2; (v) -x + 1, -y + 1, -z + 1; (vi) x - 1/2, -y + 1/2, z - 1/2; (vii) -x + 3/2, y + 1/2, -z + 3/2.]

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Crystal data

$C_{17}H_{15}IO_2S$
M_r = 410.25
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.1034 (3) Å
b = 13.1942 (4) Å
c = 11.9933 (3) Å
β = 92.634 (1)°
V = 1597.09 (8) Å^3
Z = 4
$F(000)$ = 808
D_x = 1.706 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9921 reflections
θ = 2.3–27.5°
μ = 2.14 mm^{-1}
T = 173 K
Block, colourless
0.32 × 0.27 × 0.09 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} = 0.551, T_{max} = 0.834
15129 measured reflections
3667 independent reflections
3366 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −8→13
k = −17→10
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.069$
$S = 1.07$
3667 reflections
192 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
$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 1.5593P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.96$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ 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 $F^2 > 2$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}
I	0.491732 (16)	0.129285 (13)	1.209790 (12)	0.03433 (7)
S	0.44476 (6)	0.12571 (4)	0.57565 (5)	0.02928 (13)
O2	0.5466 (2)	0.12728 (14)	0.48973 (19)	0.0451 (5)
O1	0.36148 (16)	0.39156 (12)	0.71054 (13)	0.0269 (3)
C1	0.4080 (2)	0.25304 (17)	0.60955 (18)	0.0254 (4)
C2	0.3800 (2)	0.33516 (18)	0.53236 (19)	0.0253 (4)
C3	0.3795 (2)	0.34768 (18)	0.41673 (19)	0.0281 (5)
H3	0.3964	0.2931	0.3704	0.034*
C4	0.3531 (2)	0.44313 (19)	0.3722 (2)	0.0292 (5)
C5	0.3273 (2)	0.52457 (18)	0.4432 (2)	0.0300 (5)
H5	0.3108	0.5881	0.4120	0.036*
C6	0.3253 (2)	0.51387 (18)	0.5580 (2)	0.0290 (5)
H6	0.3068	0.5680	0.6045	0.035*
C7	0.3525 (2)	0.41812 (17)	0.59933 (18)	0.0253 (4)
C8	0.3968 (2)	0.29066 (17)	0.71460 (18)	0.0255 (4)
C9	0.4144 (2)	0.24931 (17)	0.82760 (18)	0.0261 (4)
C10	0.5115 (2)	0.1770 (2)	0.85308 (19)	0.0309 (5)
H10	0.5633	0.1525	0.7969	0.037*
C11	0.5319 (3)	0.14090 (19)	0.9612 (2)	0.0315 (5)
H11	0.5966	0.0923	0.9775	0.038*
C12	0.4547 (2)	0.17826 (18)	1.04487 (18)	0.0276 (5)
C13	0.3559 (2)	0.24893 (18)	1.02076 (19)	0.0288 (5)
H13	0.3034	0.2725	1.0769	0.035*
C14	0.3359 (2)	0.28432 (18)	0.91224 (19)	0.0283 (5)
H14	0.2697	0.3317	0.8959	0.034*

C15	0.3528 (3)	0.4598 (2)	0.2475 (2)	0.0384 (6)
H15A	0.4124	0.4127	0.2151	0.058*
H15B	0.3810	0.5278	0.2326	0.058*
H15C	0.2649	0.4496	0.2156	0.058*
C16	0.2900 (3)	0.0929 (2)	0.5052 (2)	0.0372 (6)
H16A	0.2704	0.1419	0.4465	0.045*
H16B	0.2984	0.0270	0.4705	0.045*
C17	0.1766 (3)	0.0902 (2)	0.5821 (3)	0.0486 (7)
H17A	0.1975	0.0446	0.6428	0.073*
H17B	0.0981	0.0673	0.5417	0.073*
H17C	0.1620	0.1569	0.6109	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I	0.03738 (11)	0.04108 (12)	0.02435 (9)	0.00488 (7)	−0.00062 (7)	0.00094 (6)
S	0.0299 (3)	0.0259 (3)	0.0322 (3)	0.0037 (2)	0.0021 (2)	−0.0051 (2)
O2	0.0406 (11)	0.0417 (11)	0.0547 (13)	0.0043 (8)	0.0192 (10)	−0.0043 (9)
O1	0.0306 (8)	0.0241 (8)	0.0258 (8)	0.0025 (6)	−0.0021 (6)	−0.0040 (6)
C1	0.0272 (11)	0.0226 (11)	0.0264 (10)	0.0002 (8)	0.0006 (8)	−0.0023 (8)
C2	0.0228 (10)	0.0249 (11)	0.0283 (11)	−0.0021 (9)	0.0007 (8)	−0.0019 (9)
C3	0.0284 (11)	0.0286 (11)	0.0275 (11)	−0.0032 (9)	0.0035 (9)	−0.0028 (9)
C4	0.0242 (11)	0.0340 (12)	0.0294 (11)	−0.0053 (9)	0.0023 (9)	0.0032 (9)
C5	0.0259 (11)	0.0265 (11)	0.0373 (12)	−0.0018 (9)	−0.0010 (9)	0.0042 (9)
C6	0.0267 (11)	0.0257 (11)	0.0344 (12)	0.0002 (9)	−0.0014 (9)	−0.0040 (9)
C7	0.0235 (10)	0.0271 (11)	0.0253 (10)	−0.0013 (9)	−0.0010 (8)	−0.0028 (8)
C8	0.0243 (10)	0.0242 (11)	0.0278 (10)	0.0020 (8)	−0.0005 (8)	−0.0027 (8)
C9	0.0260 (11)	0.0277 (11)	0.0244 (10)	0.0001 (9)	−0.0017 (8)	−0.0032 (8)
C10	0.0283 (12)	0.0400 (14)	0.0244 (10)	0.0086 (10)	0.0020 (9)	−0.0033 (9)
C11	0.0288 (12)	0.0362 (13)	0.0290 (11)	0.0079 (10)	−0.0031 (9)	−0.0034 (9)
C12	0.0293 (11)	0.0298 (12)	0.0234 (10)	−0.0015 (9)	−0.0014 (9)	−0.0037 (9)
C13	0.0308 (12)	0.0295 (12)	0.0265 (11)	0.0034 (9)	0.0035 (9)	−0.0048 (9)
C14	0.0280 (11)	0.0258 (11)	0.0310 (11)	0.0049 (9)	−0.0002 (9)	−0.0032 (9)
C15	0.0434 (15)	0.0424 (15)	0.0298 (12)	−0.0048 (12)	0.0044 (10)	0.0068 (11)
C16	0.0397 (14)	0.0326 (13)	0.0392 (13)	−0.0019 (11)	−0.0007 (11)	−0.0048 (11)
C17	0.0383 (15)	0.0398 (15)	0.068 (2)	−0.0042 (12)	0.0118 (14)	−0.0039 (14)

Geometric parameters (Å, º)

I—C12	2.098 (2)	C9—C10	1.392 (3)
I—O2^{i}	3.378 (2)	C9—C14	1.395 (3)
S—O2	1.490 (2)	C10—C11	1.388 (3)
S—C1	1.772 (2)	C10—H10	0.9300
S—C16	1.796 (3)	C11—C12	1.390 (3)
O1—C7	1.378 (3)	C11—H11	0.9300
O1—C8	1.379 (3)	C12—C13	1.386 (3)
C1—C8	1.364 (3)	C13—C14	1.389 (3)
C1—C2	1.445 (3)	C13—H13	0.9300

C2—C7	1.393 (3)	C14—H14	0.9300
C2—C3	1.396 (3)	C15—H15A	0.9600
C3—C4	1.389 (3)	C15—H15B	0.9600
C3—H3	0.9300	C15—H15C	0.9600
C4—C5	1.402 (3)	C16—C17	1.503 (4)
C4—C15	1.513 (3)	C16—H16A	0.9700
C5—C6	1.386 (3)	C16—H16B	0.9700
C5—H5	0.9300	C17—H17A	0.9600
C6—C7	1.380 (3)	C17—H17B	0.9600
C6—H6	0.9300	C17—H17C	0.9600
C8—C9	1.464 (3)		

C12—I—O2^{i}	162.46 (7)	C11—C10—H10	119.6
O2—S—C1	107.71 (11)	C9—C10—H10	119.6
O2—S—C16	107.00 (13)	C10—C11—C12	119.3 (2)
C1—S—C16	98.58 (12)	C10—C11—H11	120.4
C7—O1—C8	106.57 (17)	C12—C11—H11	120.4
C8—C1—C2	107.27 (19)	C13—C12—C11	120.7 (2)
C8—C1—S	125.75 (18)	C13—C12—I	119.95 (16)
C2—C1—S	126.94 (17)	C11—C12—I	119.34 (18)
C7—C2—C3	119.2 (2)	C12—C13—C14	119.6 (2)
C7—C2—C1	104.97 (19)	C12—C13—H13	120.2
C3—C2—C1	135.8 (2)	C14—C13—H13	120.2
C4—C3—C2	118.7 (2)	C13—C14—C9	120.5 (2)
C4—C3—H3	120.6	C13—C14—H14	119.8
C2—C3—H3	120.6	C9—C14—H14	119.8
C3—C4—C5	120.0 (2)	C4—C15—H15A	109.5
C3—C4—C15	120.3 (2)	C4—C15—H15B	109.5
C5—C4—C15	119.8 (2)	H15A—C15—H15B	109.5
C6—C5—C4	122.4 (2)	C4—C15—H15C	109.5
C6—C5—H5	118.8	H15A—C15—H15C	109.5
C4—C5—H5	118.8	H15B—C15—H15C	109.5
C7—C6—C5	116.0 (2)	C17—C16—S	112.9 (2)
C7—C6—H6	122.0	C17—C16—H16A	109.0
C5—C6—H6	122.0	S—C16—H16A	109.0
O1—C7—C6	125.7 (2)	C17—C16—H16B	109.0
O1—C7—C2	110.6 (2)	S—C16—H16B	109.0
C6—C7—C2	123.6 (2)	H16A—C16—H16B	107.8
C1—C8—O1	110.56 (19)	C16—C17—H17A	109.5
C1—C8—C9	135.1 (2)	C16—C17—H17B	109.5
O1—C8—C9	114.37 (18)	H17A—C17—H17B	109.5
C10—C9—C14	119.0 (2)	C16—C17—H17C	109.5
C10—C9—C8	120.9 (2)	H17A—C17—H17C	109.5
C14—C9—C8	120.1 (2)	H17B—C17—H17C	109.5
C11—C10—C9	120.9 (2)		

O2—S—C1—C8	−134.9 (2)	C2—C1—C8—O1	0.8 (3)
C16—S—C1—C8	114.1 (2)	S—C1—C8—O1	−177.22 (16)

O2—S—C1—C2	47.4 (2)	C2—C1—C8—C9	−178.6 (2)
C16—S—C1—C2	−63.6 (2)	S—C1—C8—C9	3.3 (4)
C8—C1—C2—C7	−0.4 (3)	C7—O1—C8—C1	−1.0 (2)
S—C1—C2—C7	177.68 (17)	C7—O1—C8—C9	178.56 (19)
C8—C1—C2—C3	177.1 (3)	C1—C8—C9—C10	34.9 (4)
S—C1—C2—C3	−4.8 (4)	O1—C8—C9—C10	−144.5 (2)
C7—C2—C3—C4	0.8 (3)	C1—C8—C9—C14	−146.9 (3)
C1—C2—C3—C4	−176.4 (2)	O1—C8—C9—C14	33.7 (3)
C2—C3—C4—C5	−0.2 (3)	C14—C9—C10—C11	−1.0 (4)
C2—C3—C4—C15	179.5 (2)	C8—C9—C10—C11	177.2 (2)
C3—C4—C5—C6	−0.7 (4)	C9—C10—C11—C12	−0.4 (4)
C15—C4—C5—C6	179.6 (2)	C10—C11—C12—C13	1.6 (4)
C4—C5—C6—C7	1.0 (3)	C10—C11—C12—I	−176.97 (19)
C8—O1—C7—C6	−176.9 (2)	C11—C12—C13—C14	−1.4 (4)
C8—O1—C7—C2	0.8 (2)	I—C12—C13—C14	177.17 (18)
C5—C6—C7—O1	177.0 (2)	C12—C13—C14—C9	0.0 (4)
C5—C6—C7—C2	−0.3 (3)	C10—C9—C14—C13	1.2 (4)
C3—C2—C7—O1	−178.3 (2)	C8—C9—C14—C13	−177.1 (2)
C1—C2—C7—O1	−0.3 (2)	O2—S—C16—C17	−179.0 (2)
C3—C2—C7—C6	−0.6 (4)	C1—S—C16—C17	−67.5 (2)
C1—C2—C7—C6	177.4 (2)		

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

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*
C16—H16*B*···O2^{ii}	0.97	2.60	3.341 (3)	134
C11—H11···*Cg*^{iii}	0.93	2.61	3.378 (3)	141

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