Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(3-Chlorophenylsulfonyl)-5-isopropyl-2-methyl-1-benzofuran

Hong Dae Choi,[a] Pil Ja Seo[a] and Uk Lee[b]*

[a]Department of Chemistry, Dongeui University, San 24 Kaya-dong Busanjin-gu, Busan 614-714, Republic of Korea, and [b]Department of Chemistry, Pukyong National University, 599-1 Daeyeon 3-dong, Nam-gu, Busan 608-737, Republic of Korea
Correspondence e-mail: uklee@pknu.ac.kr

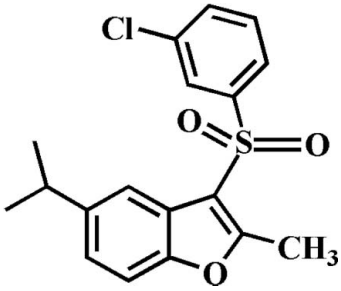
Received 21 February 2012; accepted 26 February 2012

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.132; data-to-parameter ratio = 20.1.

In the title compound, $C_{18}H_{17}ClO_3S$, the 3-chlorobenzene ring makes a dihedral angle of 82.04 (5)° with the mean plane [r.m.s. deviation = 0.006 (1) Å] of the benzofuran fragment. In the crystal, molecules are linked by weak C—H···O and C—H···π interactions.

Related literature

For background information and the crystal structures of related compounds, see: Choi *et al.* (2010, 2011).



Experimental

Crystal data

$C_{18}H_{17}ClO_3S$ M_r = 348.83
Triclinic, $P\overline{1}$
a = 7.1700 (2) Å
b = 9.9400 (2) Å
c = 12.2508 (3) Å
α = 83.484 (1)°
β = 77.907 (1)°
γ = 85.707 (1)°
V = 847.05 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 173 K
0.29 × 0.24 × 0.13 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.903, T_{max} = 0.955
16044 measured reflections
4231 independent reflections
3596 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.132
S = 1.06
4231 reflections
211 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 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
C5—H5···O3^{i}	0.95	2.42	3.321 (2)	159
C12—H12A···O2^{ii}	0.98	2.42	3.375 (2)	165
C16—H16···Cg^{iii}	0.95	2.71	3.646 (2)	170

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

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LR2052).

References

Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2009). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Choi, H. D., Seo, P. J. & Lee, U. (2011). *Acta Cryst.* E**67**, o1226.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2010). *Acta Cryst.* E**66**, o1067.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2012). E**68**, o942 [https://doi.org/10.1107/S1600536812008525]

3-(3-Chlorophenylsulfonyl)-5-isopropyl-2-methyl-1-benzofuran

Hong Dae Choi, Pil Ja Seo and Uk Lee

S1. Comment

As a part of our ongoing study of 5-isopropyl-2-methyl-1-benzofuran derivatives containing either 3-(4-fluorophenylsulfonyl) (Choi *et al.*, 2010) or 3-(4-chlorophenylsufonyl) (Choi *et al.*, 2011) 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 0.006 (1) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle between the 3-chlorobenzene ring and the mean plane of the benzofuran fragment is 82.04 (5)°. The crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds (Fig. 2 & Table 1). The crystal packing is further stabilized by intermolecular C—H···π interactions (Fig. 2 & Table 1, Cg is the centroid of the C2–C7 benzene ring).

S2. Experimental

77% 3-Chloroperoxybenzoic acid (381 mg, 1.7 mmol) was added in small portions to a stirred solution of 3-(3-chlorophenylsulfanyl)-5-isopropyl-2-methyl-1-benzofuran (279 mg, 0.8 mmol) in dichloromethane (30 mL) at 273 K. After being stirred at room temperature for 8h, 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, 4:1 v/v) to afford the title compound as a colorless solid [yield 70%, m.p. 357–358 K; R_f = 0.51 (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 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 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.

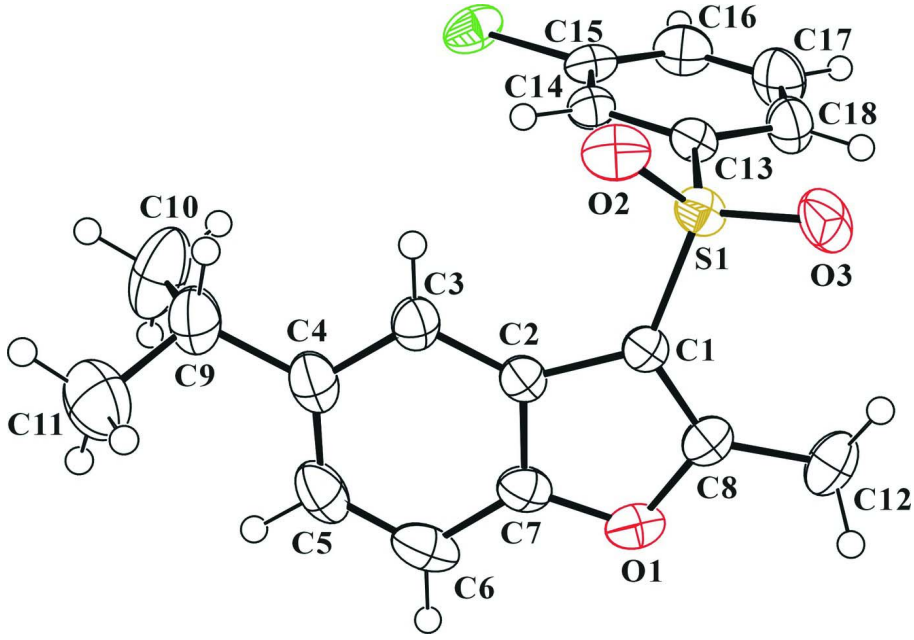


Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

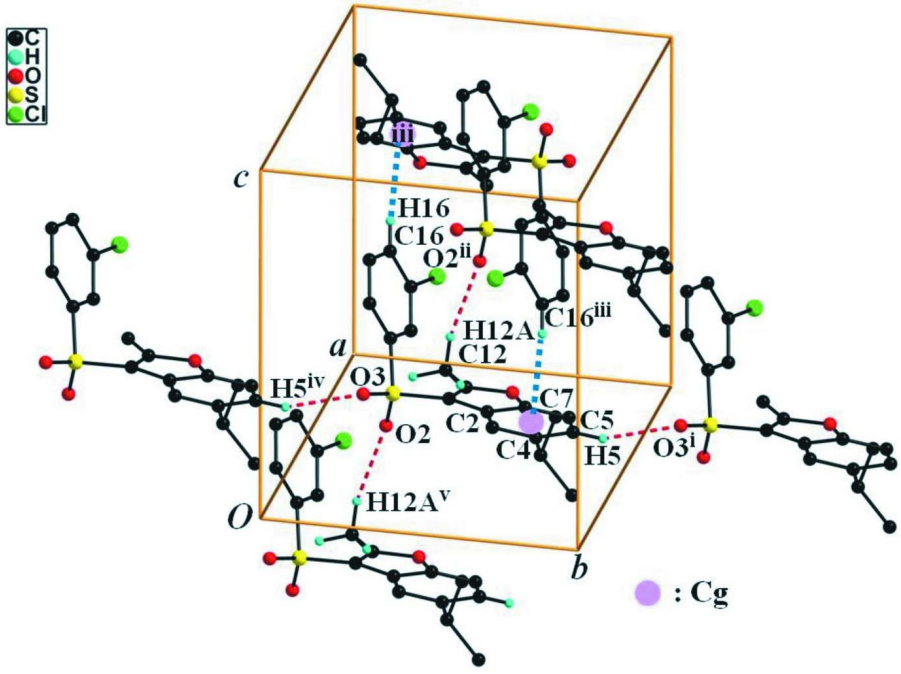


Figure 2

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

3-(3-Chlorophenylsulfonyl)-5-isopropyl-2-methyl-1-benzofuran

Crystal data

$C_{18}H_{17}ClO_3S$
$M_r = 348.83$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.1700$ (2) Å
$b = 9.9400$ (2) Å
$c = 12.2508$ (3) Å
$\alpha = 83.484$ (1)°
$\beta = 77.907$ (1)°
$\gamma = 85.707$ (1)°
$V = 847.05$ (4) Å^3
$Z = 2$
$F(000) = 364$
$D_x = 1.368$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7011 reflections
$\theta = 2.6$–$28.4°$
$\mu = 0.36$ mm^{-1}
$T = 173$ K
Block, colourless
0.29 × 0.24 × 0.13 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)
$T_{min} = 0.903$, $T_{max} = 0.955$
16044 measured reflections
4231 independent reflections
3596 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 28.4°$, $\theta_{min} = 1.7°$
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.132$
$S = 1.06$
4231 reflections
211 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
$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.4272P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.85$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.22055 (7)	0.49026 (6)	0.63396 (4)	0.04596 (16)
S1	0.34765 (7)	0.31464 (4)	0.22246 (3)	0.03083 (13)
O1	0.71701 (19)	0.58220 (14)	0.07545 (10)	0.0376 (3)

O2	0.1494 (2)	0.35118 (15)	0.22738 (12)	0.0418 (3)
O3	0.4313 (3)	0.19619 (14)	0.17075 (12)	0.0470 (4)
C1	0.4757 (2)	0.45364 (16)	0.16032 (13)	0.0269 (3)
C2	0.4074 (3)	0.59381 (16)	0.16760 (13)	0.0287 (3)
C3	0.2339 (3)	0.66147 (18)	0.21091 (15)	0.0350 (4)
H3	0.1263	0.6116	0.2471	0.042*
C4	0.2210 (3)	0.8016 (2)	0.20043 (17)	0.0424 (5)
C5	0.3805 (4)	0.8721 (2)	0.14704 (18)	0.0485 (5)
H5	0.3705	0.9684	0.1413	0.058*
C6	0.5538 (4)	0.8085 (2)	0.10175 (18)	0.0476 (5)
H6	0.6607	0.8585	0.0645	0.057*
C7	0.5627 (3)	0.66778 (19)	0.11380 (14)	0.0346 (4)
C8	0.6615 (3)	0.45245 (18)	0.10554 (14)	0.0314 (4)
C9	0.0286 (4)	0.8735 (2)	0.2472 (2)	0.0510 (5)
H9	−0.0715	0.8055	0.2589	0.061*
C10	0.0305 (5)	0.9199 (4)	0.3600 (2)	0.0800 (10)
H10A	0.1277	0.9867	0.3513	0.120*
H10B	0.0601	0.8419	0.4112	0.120*
H10C	−0.0952	0.9612	0.3907	0.120*
C11	−0.0257 (5)	0.9892 (3)	0.1681 (3)	0.0735 (8)
H11A	−0.1572	1.0223	0.1965	0.110*
H11B	−0.0162	0.9582	0.0939	0.110*
H11C	0.0608	1.0626	0.1622	0.110*
C12	0.8097 (3)	0.3445 (2)	0.07479 (18)	0.0445 (5)
H12A	0.8950	0.3338	0.1285	0.067*
H12B	0.8836	0.3690	−0.0008	0.067*
H12C	0.7490	0.2590	0.0763	0.067*
C13	0.3857 (3)	0.29535 (17)	0.36169 (14)	0.0301 (3)
C14	0.2933 (2)	0.38686 (17)	0.43515 (14)	0.0300 (3)
H14	0.2060	0.4559	0.4127	0.036*
C15	0.3317 (3)	0.3750 (2)	0.54204 (14)	0.0337 (4)
C16	0.4560 (3)	0.2732 (2)	0.57601 (17)	0.0448 (5)
H16	0.4809	0.2661	0.6497	0.054*
C17	0.5430 (4)	0.1826 (2)	0.50199 (19)	0.0509 (5)
H17	0.6268	0.1117	0.5254	0.061*
C18	0.5105 (3)	0.1929 (2)	0.39347 (17)	0.0425 (4)
H18	0.5727	0.1309	0.3422	0.051*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0426 (3)	0.0637 (3)	0.0318 (2)	−0.0110 (2)	0.00138 (19)	−0.0171 (2)
S1	0.0390 (2)	0.0288 (2)	0.0274 (2)	−0.00753 (17)	−0.00952 (17)	−0.00579 (15)
O1	0.0365 (7)	0.0478 (8)	0.0290 (6)	−0.0133 (6)	−0.0028 (5)	−0.0056 (6)
O2	0.0366 (7)	0.0537 (8)	0.0395 (7)	−0.0132 (6)	−0.0144 (6)	−0.0029 (6)
O3	0.0747 (11)	0.0293 (6)	0.0396 (7)	−0.0061 (7)	−0.0112 (7)	−0.0126 (6)
C1	0.0312 (8)	0.0283 (7)	0.0227 (7)	−0.0026 (6)	−0.0075 (6)	−0.0047 (6)
C2	0.0369 (9)	0.0279 (8)	0.0223 (7)	−0.0019 (7)	−0.0080 (6)	−0.0036 (6)

C3	0.0419 (10)	0.0341 (9)	0.0295 (8)	0.0035 (7)	−0.0087 (7)	−0.0057 (7)
C4	0.0611 (13)	0.0339 (9)	0.0339 (9)	0.0078 (9)	−0.0154 (9)	−0.0060 (7)
C5	0.0783 (16)	0.0285 (9)	0.0412 (11)	0.0013 (10)	−0.0184 (11)	−0.0053 (8)
C6	0.0684 (15)	0.0405 (10)	0.0359 (10)	−0.0230 (10)	−0.0118 (10)	0.0035 (8)
C7	0.0452 (10)	0.0355 (9)	0.0241 (8)	−0.0089 (8)	−0.0070 (7)	−0.0032 (6)
C8	0.0336 (9)	0.0399 (9)	0.0230 (7)	−0.0023 (7)	−0.0084 (6)	−0.0084 (7)
C9	0.0598 (14)	0.0427 (11)	0.0509 (12)	0.0112 (10)	−0.0137 (11)	−0.0104 (9)
C10	0.0746 (19)	0.110 (3)	0.0598 (16)	0.0405 (18)	−0.0238 (15)	−0.0397 (17)
C11	0.0756 (19)	0.0659 (17)	0.080 (2)	0.0106 (15)	−0.0291 (16)	0.0048 (15)
C12	0.0342 (10)	0.0599 (13)	0.0421 (10)	0.0094 (9)	−0.0111 (8)	−0.0176 (9)
C13	0.0352 (9)	0.0282 (8)	0.0275 (8)	−0.0057 (7)	−0.0076 (7)	−0.0010 (6)
C14	0.0290 (8)	0.0333 (8)	0.0284 (8)	−0.0054 (7)	−0.0060 (6)	−0.0035 (6)
C15	0.0316 (9)	0.0432 (10)	0.0258 (8)	−0.0117 (7)	−0.0018 (7)	−0.0031 (7)
C16	0.0506 (12)	0.0543 (12)	0.0317 (9)	−0.0072 (10)	−0.0153 (9)	0.0032 (8)
C17	0.0606 (14)	0.0468 (12)	0.0465 (12)	0.0093 (10)	−0.0224 (11)	0.0039 (9)
C18	0.0513 (12)	0.0353 (9)	0.0404 (10)	0.0065 (8)	−0.0114 (9)	−0.0040 (8)

Geometric parameters (Å, º)

Cl1—C15	1.7307 (19)	C9—C10	1.509 (4)
S1—O2	1.4308 (15)	C9—H9	1.0000
S1—O3	1.4325 (14)	C10—H10A	0.9800
S1—C1	1.7290 (17)	C10—H10B	0.9800
S1—C13	1.7700 (18)	C10—H10C	0.9800
O1—C8	1.366 (2)	C11—H11A	0.9800
O1—C7	1.379 (2)	C11—H11B	0.9800
C1—C8	1.360 (2)	C11—H11C	0.9800
C1—C2	1.448 (2)	C12—H12A	0.9800
C2—C7	1.386 (3)	C12—H12B	0.9800
C2—C3	1.400 (2)	C12—H12C	0.9800
C3—C4	1.382 (3)	C13—C18	1.382 (3)
C3—H3	0.9500	C13—C14	1.386 (2)
C4—C5	1.389 (3)	C14—C15	1.384 (2)
C4—C9	1.534 (3)	C14—H14	0.9500
C5—C6	1.387 (3)	C15—C16	1.385 (3)
C5—H5	0.9500	C16—C17	1.374 (3)
C6—C7	1.387 (3)	C16—H16	0.9500
C6—H6	0.9500	C17—C18	1.388 (3)
C8—C12	1.475 (3)	C17—H17	0.9500
C9—C11	1.501 (3)	C18—H18	0.9500
O2—S1—O3	119.69 (9)	C9—C10—H10A	109.5
O2—S1—C1	107.76 (8)	C9—C10—H10B	109.5
O3—S1—C1	109.52 (9)	H10A—C10—H10B	109.5
O2—S1—C13	107.50 (8)	C9—C10—H10C	109.5
O3—S1—C13	107.43 (9)	H10A—C10—H10C	109.5
C1—S1—C13	103.79 (8)	H10B—C10—H10C	109.5
C8—O1—C7	107.30 (14)	C9—C11—H11A	109.5

C8—C1—C2	107.79 (15)	C9—C11—H11B	109.5
C8—C1—S1	126.80 (14)	H11A—C11—H11B	109.5
C2—C1—S1	125.15 (13)	C9—C11—H11C	109.5
C7—C2—C3	119.77 (16)	H11A—C11—H11C	109.5
C7—C2—C1	104.46 (16)	H11B—C11—H11C	109.5
C3—C2—C1	135.75 (17)	C8—C12—H12A	109.5
C4—C3—C2	119.30 (19)	C8—C12—H12B	109.5
C4—C3—H3	120.3	H12A—C12—H12B	109.5
C2—C3—H3	120.3	C8—C12—H12C	109.5
C3—C4—C5	119.2 (2)	H12A—C12—H12C	109.5
C3—C4—C9	118.4 (2)	H12B—C12—H12C	109.5
C5—C4—C9	122.43 (19)	C18—C13—C14	121.69 (17)
C6—C5—C4	123.05 (18)	C18—C13—S1	119.55 (14)
C6—C5—H5	118.5	C14—C13—S1	118.73 (14)
C4—C5—H5	118.5	C15—C14—C13	118.22 (17)
C7—C6—C5	116.5 (2)	C15—C14—H14	120.9
C7—C6—H6	121.8	C13—C14—H14	120.9
C5—C6—H6	121.8	C14—C15—C16	121.22 (18)
O1—C7—C2	110.48 (15)	C14—C15—Cl1	118.77 (15)
O1—C7—C6	127.30 (18)	C16—C15—Cl1	120.01 (15)
C2—C7—C6	122.21 (19)	C17—C16—C15	119.26 (19)
C1—C8—O1	109.96 (15)	C17—C16—H16	120.4
C1—C8—C12	134.29 (18)	C15—C16—H16	120.4
O1—C8—C12	115.74 (16)	C16—C17—C18	121.1 (2)
C11—C9—C10	111.0 (2)	C16—C17—H17	119.5
C11—C9—C4	112.9 (2)	C18—C17—H17	119.5
C10—C9—C4	110.2 (2)	C13—C18—C17	118.53 (19)
C11—C9—H9	107.5	C13—C18—H18	120.7
C10—C9—H9	107.5	C17—C18—H18	120.7
C4—C9—H9	107.5		

O2—S1—C1—C8	−156.03 (15)	S1—C1—C8—O1	−175.31 (11)
O3—S1—C1—C8	−24.32 (18)	C2—C1—C8—C12	178.02 (19)
C13—S1—C1—C8	90.16 (16)	S1—C1—C8—C12	3.6 (3)
O2—S1—C1—C2	30.48 (16)	C7—O1—C8—C1	0.90 (19)
O3—S1—C1—C2	162.19 (14)	C7—O1—C8—C12	−178.25 (15)
C13—S1—C1—C2	−83.33 (16)	C3—C4—C9—C11	−135.1 (2)
C8—C1—C2—C7	0.54 (18)	C5—C4—C9—C11	44.1 (3)
S1—C1—C2—C7	175.07 (13)	C3—C4—C9—C10	100.2 (3)
C8—C1—C2—C3	178.83 (19)	C5—C4—C9—C10	−80.7 (3)
S1—C1—C2—C3	−6.6 (3)	O2—S1—C13—C18	141.75 (16)
C7—C2—C3—C4	−0.7 (3)	O3—S1—C13—C18	11.71 (19)
C1—C2—C3—C4	−178.83 (18)	C1—S1—C13—C18	−104.25 (17)
C2—C3—C4—C5	0.0 (3)	O2—S1—C13—C14	−40.32 (16)
C2—C3—C4—C9	179.19 (17)	O3—S1—C13—C14	−170.36 (14)
C3—C4—C5—C6	0.9 (3)	C1—S1—C13—C14	73.68 (15)
C9—C4—C5—C6	−178.2 (2)	C18—C13—C14—C15	1.1 (3)
C4—C5—C6—C7	−1.1 (3)	S1—C13—C14—C15	−176.74 (13)

C8—O1—C7—C2	−0.54 (19)	C13—C14—C15—C16	−1.2 (3)
C8—O1—C7—C6	−179.70 (19)	C13—C14—C15—Cl1	178.92 (13)
C3—C2—C7—O1	−178.62 (15)	C14—C15—C16—C17	0.1 (3)
C1—C2—C7—O1	0.00 (19)	Cl1—C15—C16—C17	−179.99 (17)
C3—C2—C7—C6	0.6 (3)	C15—C16—C17—C18	1.0 (4)
C1—C2—C7—C6	179.21 (17)	C14—C13—C18—C17	0.0 (3)
C5—C6—C7—O1	179.36 (18)	S1—C13—C18—C17	177.84 (17)
C5—C6—C7—C2	0.3 (3)	C16—C17—C18—C13	−1.1 (4)
C2—C1—C8—O1	−0.90 (19)		

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*
C5—H5···O3^{i}	0.95	2.42	3.321 (2)	159
C12—H12*A*···O2^{ii}	0.98	2.42	3.375 (2)	165
C16—H16···*Cg*^{iii}	0.95	2.71	3.646 (2)	170

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