Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-Chloro-3-cyclohexylsulfonyl-2-methyl-1-benzofuran

Hong Dae Choi,[a] Pil Ja Seo,[a] Byeng Wha Son[b] 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

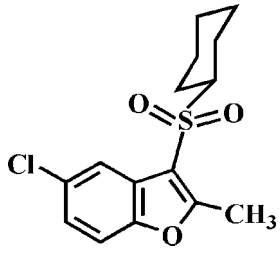
Received 17 February 2011; accepted 4 March 2011

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.093; data-to-parameter ratio = 18.1.

In the title compound, $C_{15}H_{17}ClO_3S$, the cyclohexyl ring adopts a chair conformation. In the crystal, molecules are linked through weak intermolecular C—H···O and C—H···π interactions.

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 structural studies of related 3-arylsulfonyl-5-chloro-2-methyl-1-benzofuran derivatives, see: Choi *et al.* (2008, 2010).



Experimental

Crystal data

$C_{15}H_{17}ClO_3S$
M_r = 312.80
Monoclinic, $P2_1/c$
a = 14.3135 (2) Å
b = 9.2829 (2) Å
c = 11.3433 (2) Å
β = 107.566 (1)°
V = 1436.91 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 173 K
0.29 × 0.18 × 0.11 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.891, T_{max} = 0.954
13251 measured reflections
3287 independent reflections
2856 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.093
S = 1.07
3287 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

Cg is the centroid of the benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O3^{i}	0.95	2.54	3.2630 (19)	133
C10—H10···O2^{ii}	1.00	2.42	3.3899 (19)	162
C9—H9*C*···*Cg*^{iii}	0.98	2.69	3.577 (2)	151

Symmetry codes: (i) $x, y-1, z$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (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: BH2340).

References

Akgul, Y. Y. & Anil, H. (2003). *Phytochemistry*, **63**, 939–943.
Aslam, S. N., Stevenson, P. C., Phythian, S. J., Veitch, N. C. & Hall, D. R. (2006). *Tetrahedron*, **62**, 4214–4226.
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., Son, B. W. & Lee, U. (2008). *Acta Cryst.* E**64**, o1190.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2010). *Acta Cryst.* E**66**, o2350.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Galal, S. A., Abd El-All, A. S., Abdallah, M. M. & El-Diwani, H. I. (2009). *Bioorg. Med. Chem. Lett.* **19**, 2420–2428.
Khan, M. W., Alam, M. J., Rashid, M. A. & Chowdhury, R. (2005). *Bioorg. Med. Chem.* **13**, 4796–4805.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Soekamto, N. H., Achmad, S. A., Ghisalberti, E. L., Hakim, E. H. & Syah, Y. M. (2003). *Phytochemistry*, **64**, 831–834.

supporting information

Acta Cryst. (2011). E**67**, o828 [doi:10.1107/S1600536811008270]

5-Chloro-3-cyclohexylsulfonyl-2-methyl-1-benzofuran

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

S1. Comment

Many compounds containing a benzofuran ring exhibit interesting pharmacological properties such as antifungal, antitumor and antiviral, and antimicrobial activities (Aslam *et al.*, 2006; Galal *et al.*, 2009; Khan *et al.*, 2005). These compounds occur in a wide range of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing study of the substituent effect on the solid state structures of 3-arylsulfonyl-5-chloro-2-methyl-1-benzofuran analogues (Choi *et al.*, 2008, 2010), 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 (1) Å from the least-squares plane defined by the nine constituent atoms. The cyclohexyl ring is in the chair form. The molecular packing (Fig. 2) is stabilized by weak intermolecular C–H···O hydrogen bonds; the first one between a benzene H atom and the O atom of the sulfonyl unit (Table 1: C6–H6···O3^{i}), and the second one between a cyclohexyl H atom and the O atom of the sulfonyl unit (Table 1: C10–H10···O2^{ii}). The crystal packing (Fig. 2) is further stabilized by intermolecular C–H···π interactions between a methyl H atoms and the benzene rings (Table 1: C9–H9C···Cg^{iii}, Cg is the centroid of the C2···C7 benzene ring).

S2. Experimental

77% 3-chloroperoxybenzoic acid (515 mg, 2.3 mmol) was added in small portions to a stirred solution of 5-chloro-3-cyclohexylsulfanyl-2-methyl-1-benzofuran (389 mg, 1.1 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 5 h, 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 73%, m.p. 440-441 K; R_f = 0.63 (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, 1.00 Å for methine, 0.99 Å for methylene and 0.98 Å for methyl H atoms, respectively. U_{iso}(H) = 1.2U_{eq}(C) for aryl, methine and methylene, and 1.5U_{eq}(C) for methyl H atoms.

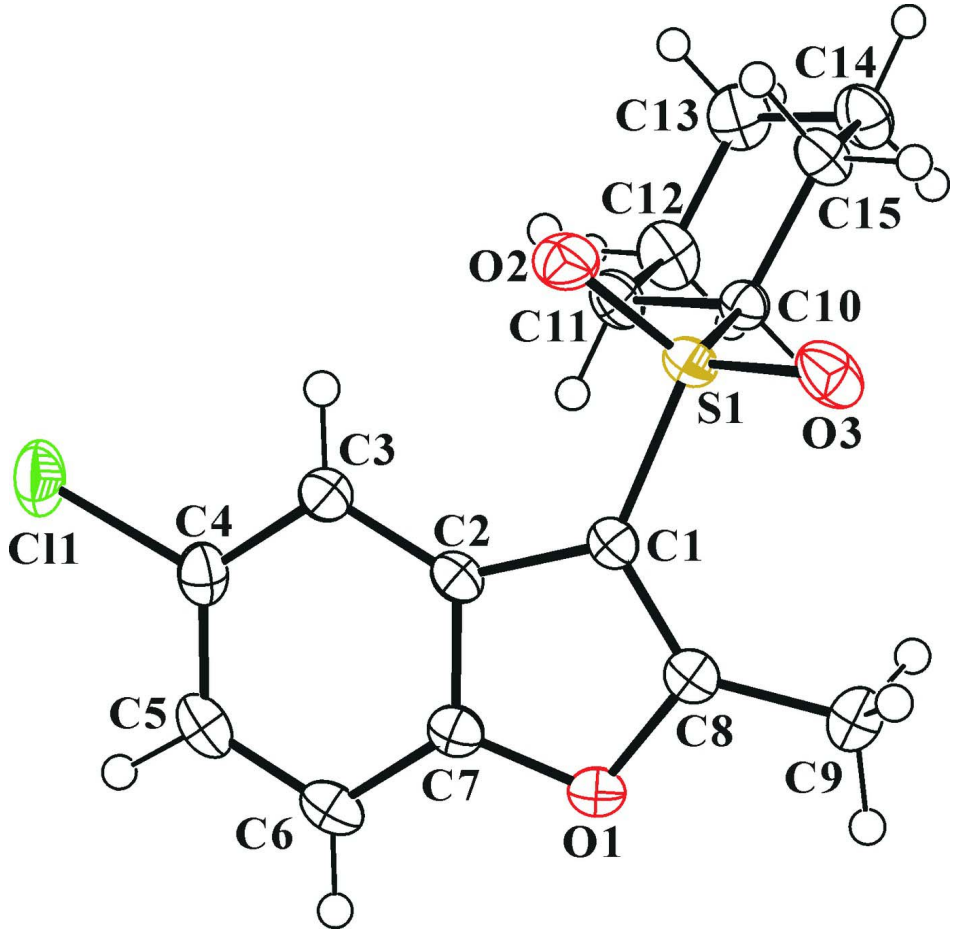


Figure 1

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

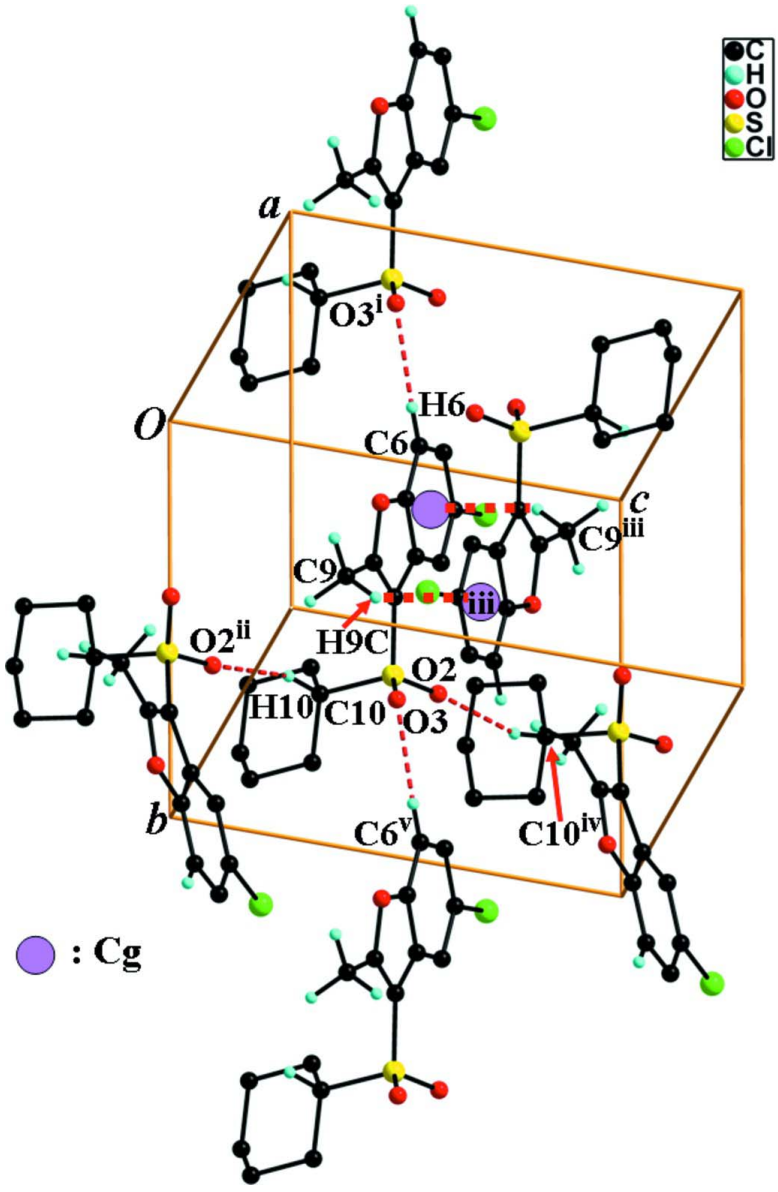


Figure 2

A view of the C–H···O and C–H···π interactions (dotted lines) in the crystal structure of the title compound [Symmetry codes: (i) x, y-1, z; (ii) x, -y+3/2, z-1/2; (iii) -x+1, -y+1, -z+1; (iv) x, -y+3/2, z+1/2; (v) x, y+1, z].

5-Chloro-3-cyclohexylsulfonyl-2-methyl-1-benzofuran

Crystal data

$C_{15}H_{17}ClO_3S$
M_r = 312.80
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 14.3135 (2) Å
b = 9.2829 (2) Å
c = 11.3433 (2) Å
β = 107.566 (1)°
V = 1436.91 (4) Å^3
Z = 4
F(000) = 656
D_x = 1.446 Mg m^{-3}
Melting point: 440 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5109 reflections
θ = 2.7–27.5°

μ = 0.42 mm^{-1}
T = 173 K

Block, colourless
0.29 × 0.18 × 0.11 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} = 0.891, T_{max} = 0.954

13251 measured reflections
3287 independent reflections
2856 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°, θ_{min} = 1.5°
h = −18→18
k = −12→10
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.093
S = 1.07
3287 reflections
182 parameters
0 restraints
0 constraints

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
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.5583P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S	0.31521 (3)	0.72877 (4)	0.40822 (3)	0.02105 (11)
Cl	0.18841 (3)	0.20832 (5)	0.64837 (4)	0.03919 (13)
O2	0.28307 (9)	0.73602 (12)	0.51704 (10)	0.0298 (3)
O1	0.43749 (7)	0.36827 (12)	0.34930 (10)	0.0255 (2)
O3	0.38824 (8)	0.82960 (12)	0.39699 (11)	0.0320 (3)
C1	0.35822 (10)	0.55463 (15)	0.40040 (13)	0.0208 (3)
C2	0.33118 (10)	0.42681 (15)	0.45538 (13)	0.0209 (3)
C3	0.27018 (10)	0.39605 (17)	0.52741 (14)	0.0242 (3)
H3	0.2347	0.4694	0.5537	0.029*
C4	0.26403 (11)	0.25316 (18)	0.55855 (15)	0.0266 (3)
C5	0.31494 (11)	0.14251 (17)	0.52184 (15)	0.0294 (3)
H5	0.3075	0.0459	0.5452	0.035*
C6	0.37639 (11)	0.17320 (17)	0.45146 (15)	0.0284 (3)
H6	0.4125	0.1000	0.4260	0.034*
C7	0.38230 (10)	0.31567 (16)	0.42022 (14)	0.0230 (3)
C8	0.42122 (10)	0.51346 (16)	0.33784 (13)	0.0226 (3)
C9	0.47360 (11)	0.59044 (18)	0.26251 (15)	0.0292 (3)
H9A	0.4262	0.6427	0.1956	0.044*
H9B	0.5091	0.5208	0.2272	0.044*
H9C	0.5201	0.6588	0.3148	0.044*
C10	0.21039 (10)	0.74609 (15)	0.27476 (13)	0.0208 (3)
H10	0.2316	0.7276	0.1998	0.025*

C11	0.13094 (11)	0.63719 (17)	0.27601 (15)	0.0285 (3)
H11A	0.1104	0.6511	0.3511	0.034*
H11B	0.1570	0.5382	0.2778	0.034*
C12	0.04281 (12)	0.6570 (2)	0.16061 (17)	0.0362 (4)
H12A	0.0626	0.6364	0.0859	0.043*
H12B	−0.0094	0.5880	0.1628	0.043*
C13	0.00340 (12)	0.8095 (2)	0.15363 (18)	0.0367 (4)
H13A	−0.0523	0.8209	0.0773	0.044*
H13B	−0.0209	0.8278	0.2253	0.044*
C14	0.08265 (12)	0.91795 (19)	0.15367 (16)	0.0338 (4)
H14A	0.0561	1.0166	0.1522	0.041*
H14B	0.1027	0.9049	0.0781	0.041*
C15	0.17212 (11)	0.90049 (16)	0.26764 (15)	0.0274 (3)
H15A	0.2241	0.9684	0.2627	0.033*
H15B	0.1539	0.9231	0.3431	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.02279 (18)	0.01684 (18)	0.02228 (19)	0.00067 (12)	0.00493 (14)	−0.00147 (13)
Cl	0.0382 (2)	0.0426 (3)	0.0397 (3)	−0.00341 (17)	0.01619 (19)	0.01558 (19)
O2	0.0390 (6)	0.0287 (6)	0.0215 (5)	0.0062 (5)	0.0088 (5)	−0.0033 (4)
O1	0.0275 (5)	0.0225 (5)	0.0282 (6)	0.0036 (4)	0.0111 (4)	−0.0011 (4)
O3	0.0265 (5)	0.0208 (5)	0.0445 (7)	−0.0038 (4)	0.0044 (5)	0.0007 (5)
C1	0.0219 (6)	0.0188 (7)	0.0213 (7)	0.0000 (5)	0.0057 (5)	0.0003 (5)
C2	0.0213 (6)	0.0183 (7)	0.0206 (7)	0.0006 (5)	0.0027 (5)	0.0004 (5)
C3	0.0239 (7)	0.0243 (7)	0.0241 (7)	0.0019 (6)	0.0068 (6)	0.0015 (6)
C4	0.0235 (7)	0.0300 (8)	0.0246 (7)	−0.0025 (6)	0.0047 (6)	0.0063 (6)
C5	0.0329 (8)	0.0203 (7)	0.0302 (8)	−0.0011 (6)	0.0025 (6)	0.0050 (6)
C6	0.0305 (8)	0.0197 (7)	0.0318 (8)	0.0037 (6)	0.0045 (6)	−0.0012 (6)
C7	0.0226 (7)	0.0221 (7)	0.0227 (7)	0.0011 (5)	0.0045 (5)	−0.0011 (6)
C8	0.0220 (6)	0.0221 (7)	0.0220 (7)	−0.0001 (5)	0.0039 (5)	−0.0005 (6)
C9	0.0282 (7)	0.0339 (9)	0.0274 (8)	−0.0029 (6)	0.0114 (6)	0.0012 (7)
C10	0.0214 (7)	0.0206 (7)	0.0196 (7)	0.0007 (5)	0.0052 (5)	0.0002 (5)
C11	0.0274 (7)	0.0225 (7)	0.0326 (8)	−0.0035 (6)	0.0047 (6)	0.0011 (6)
C12	0.0282 (8)	0.0351 (9)	0.0387 (10)	−0.0083 (7)	0.0000 (7)	−0.0002 (8)
C13	0.0231 (8)	0.0417 (10)	0.0403 (10)	0.0006 (7)	0.0022 (7)	0.0053 (8)
C14	0.0286 (8)	0.0321 (9)	0.0363 (9)	0.0039 (6)	0.0030 (7)	0.0096 (7)
C15	0.0264 (7)	0.0211 (7)	0.0319 (8)	0.0014 (6)	0.0046 (6)	0.0030 (6)

Geometric parameters (Å, º)

S—O3	1.4372 (11)	C9—H9B	0.9800
S—O2	1.4431 (12)	C9—H9C	0.9800
S—C1	1.7416 (15)	C10—C11	1.525 (2)
S—C10	1.7882 (14)	C10—C15	1.528 (2)
Cl—C4	1.7461 (16)	C10—H10	1.0000
O1—C8	1.3673 (18)	C11—C12	1.530 (2)

O1—C7	1.3760 (18)	C11—H11A	0.9900
C1—C8	1.360 (2)	C11—H11B	0.9900
C1—C2	1.447 (2)	C12—C13	1.517 (3)
C2—C7	1.391 (2)	C12—H12A	0.9900
C2—C3	1.393 (2)	C12—H12B	0.9900
C3—C4	1.382 (2)	C13—C14	1.516 (2)
C3—H3	0.9500	C13—H13A	0.9900
C4—C5	1.394 (2)	C13—H13B	0.9900
C5—C6	1.384 (2)	C14—C15	1.529 (2)
C5—H5	0.9500	C14—H14A	0.9900
C6—C7	1.378 (2)	C14—H14B	0.9900
C6—H6	0.9500	C15—H15A	0.9900
C8—C9	1.480 (2)	C15—H15B	0.9900
C9—H9A	0.9800		

O3—S—O2	118.27 (7)	C11—C10—C15	111.46 (12)
O3—S—C1	108.80 (7)	C11—C10—S	111.72 (10)
O2—S—C1	107.20 (7)	C15—C10—S	108.96 (10)
O3—S—C10	108.26 (7)	C11—C10—H10	108.2
O2—S—C10	108.50 (7)	C15—C10—H10	108.2
C1—S—C10	105.04 (7)	S—C10—H10	108.2
C8—O1—C7	107.10 (11)	C10—C11—C12	109.68 (13)
C8—C1—C2	107.48 (13)	C10—C11—H11A	109.7
C8—C1—S	126.00 (11)	C12—C11—H11A	109.7
C2—C1—S	126.49 (11)	C10—C11—H11B	109.7
C7—C2—C3	119.53 (13)	C12—C11—H11B	109.7
C7—C2—C1	104.62 (13)	H11A—C11—H11B	108.2
C3—C2—C1	135.84 (13)	C13—C12—C11	110.76 (14)
C4—C3—C2	116.49 (14)	C13—C12—H12A	109.5
C4—C3—H3	121.8	C11—C12—H12A	109.5
C2—C3—H3	121.8	C13—C12—H12B	109.5
C3—C4—C5	123.47 (15)	C11—C12—H12B	109.5
C3—C4—Cl	118.45 (13)	H12A—C12—H12B	108.1
C5—C4—Cl	118.08 (12)	C14—C13—C12	110.68 (14)
C6—C5—C4	120.08 (15)	C14—C13—H13A	109.5
C6—C5—H5	120.0	C12—C13—H13A	109.5
C4—C5—H5	120.0	C14—C13—H13B	109.5
C7—C6—C5	116.40 (14)	C12—C13—H13B	109.5
C7—C6—H6	121.8	H13A—C13—H13B	108.1
C5—C6—H6	121.8	C13—C14—C15	111.43 (14)
O1—C7—C6	125.55 (14)	C13—C14—H14A	109.3
O1—C7—C2	110.42 (13)	C15—C14—H14A	109.3
C6—C7—C2	124.03 (14)	C13—C14—H14B	109.3
C1—C8—O1	110.38 (13)	C15—C14—H14B	109.3
C1—C8—C9	134.19 (14)	H14A—C14—H14B	108.0
O1—C8—C9	115.43 (13)	C10—C15—C14	109.85 (13)
C8—C9—H9A	109.5	C10—C15—H15A	109.7
C8—C9—H9B	109.5	C14—C15—H15A	109.7

H9A—C9—H9B	109.5	C10—C15—H15B	109.7
C8—C9—H9C	109.5	C14—C15—H15B	109.7
H9A—C9—H9C	109.5	H15A—C15—H15B	108.2
H9B—C9—H9C	109.5		

O3—S—C1—C8	−29.39 (15)	C3—C2—C7—C6	0.5 (2)
O2—S—C1—C8	−158.38 (13)	C1—C2—C7—C6	−178.90 (14)
C10—S—C1—C8	86.33 (14)	C2—C1—C8—O1	−0.51 (16)
O3—S—C1—C2	152.86 (12)	S—C1—C8—O1	−178.61 (10)
O2—S—C1—C2	23.87 (14)	C2—C1—C8—C9	179.31 (15)
C10—S—C1—C2	−91.41 (13)	S—C1—C8—C9	1.2 (3)
C8—C1—C2—C7	0.17 (16)	C7—O1—C8—C1	0.64 (16)
S—C1—C2—C7	178.26 (11)	C7—O1—C8—C9	−179.21 (12)
C8—C1—C2—C3	−179.09 (16)	O3—S—C10—C11	177.11 (11)
S—C1—C2—C3	−1.0 (2)	O2—S—C10—C11	−53.37 (12)
C7—C2—C3—C4	−0.6 (2)	C1—S—C10—C11	61.01 (12)
C1—C2—C3—C4	178.57 (15)	O3—S—C10—C15	−59.29 (12)
C2—C3—C4—C5	0.0 (2)	O2—S—C10—C15	70.23 (12)
C2—C3—C4—Cl	−179.83 (11)	C1—S—C10—C15	−175.40 (10)
C3—C4—C5—C6	0.7 (2)	C15—C10—C11—C12	57.47 (17)
Cl—C4—C5—C6	−179.44 (12)	S—C10—C11—C12	179.64 (12)
C4—C5—C6—C7	−0.8 (2)	C10—C11—C12—C13	−57.59 (19)
C8—O1—C7—C6	178.58 (14)	C11—C12—C13—C14	57.6 (2)
C8—O1—C7—C2	−0.52 (16)	C12—C13—C14—C15	−56.9 (2)
C5—C6—C7—O1	−178.78 (14)	C11—C10—C15—C14	−56.53 (17)
C5—C6—C7—C2	0.2 (2)	S—C10—C15—C14	179.73 (11)
C3—C2—C7—O1	179.63 (12)	C13—C14—C15—C10	55.92 (19)
C1—C2—C7—O1	0.21 (16)		

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O3^{i}	0.95	2.54	3.2630 (19)	133
C10—H10···O2^{ii}	1.00	2.42	3.3899 (19)	162
C9—H9*C*···*Cg*^{iii}	0.98	2.69	3.577 (2)	151

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, −*y*+3/2, *z*−1/2; (iii) −*x*+1, −*y*+1, −*z*+1.