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# 3-(4-Chlorophenylsulfonyl)-2,5-dimethyl-1-benzofuran

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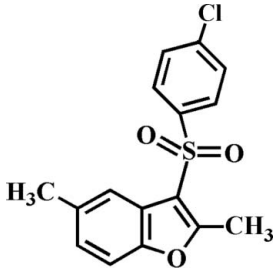
Key indicators: single-crystal X-ray study; $T$ = 177 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.040; $wR$ factor = 0.107; data-to-parameter ratio = 17.7.

In the title compound, $C_{16}H_{13}ClO_3S$, the 4-chlorophenyl ring makes a dihedral angle of 79.96 (5)° with the mean plane of the benzofuran fragment. In the crystal, molecules are linked through weak intermolecular C—H···O and C—H···$\pi$ interactions.

## Related literature

For the biological 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 our previous structural studies of related 3-(4-chlorophenylsulfinyl)-2,5-dimethyl-1-benzofuran derivatives, see: Choi *et al.* (2010*a*,*b*).




## Experimental

### Crystal data

$C_{16}H_{13}ClO_3S$
$M_r$ = 320.77
Monoclinic, $P2_1/c$
$a$ = 15.3529 (3) Å
$b$ = 12.1495 (2) Å
$c$ = 8.2663 (2) Å
$\beta$ = 105.363 (1)°
$V$ = 1486.82 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.40 mm$^{-1}$
$T$ = 177 K
0.37 × 0.23 × 0.10 mm

### Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.867, $T_{max}$ = 0.962
13864 measured reflections
3398 independent reflections
2655 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
$S$ = 1.06
3398 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.34 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···$A$ |
|---|---|---|---|---|
| C6—H6···O1$^{i}$ | 0.95 | 2.56 | 3.495 (2) | 167 |
| C10—H10$A$···O2$^{ii}$ | 0.98 | 2.43 | 3.279 (2) | 145 |
| C13—H13···$Cg^{iii}$ | 0.95 | 2.74 | 3.411 (2) | 128 |

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5054).

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# supporting information

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## 3-(4-Chlorophenylsulfonyl)-2,5-dimethyl-1-benzofuran

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

### S1. Comment

A series of benzofuran ring system has received much attention in view of their particular pharmacological properties such as antifungal, antimicrobial, antitumor and antiviral activities (Aslam *et al.*, 2006; Galal *et al.*, 2009; Khan *et al.*, 2005). These compounds widely occur in nature (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our study of the substituent effect on the solid state structures of 3-(4-chlorophenylsulfinyl)-2,5-dimethyl-1-benzofuran analogues (Choi *et al.*, 2010*a,b*), we report herein on the crystal structure of the title compound.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.003 (1 ) Å from the least-squares plane defined by the nine constituent atoms. The 4-chlorophenyl ring makes a dihedral angle of 79.96 (5)° with the mean plane of the benzofuran ring. The crystal packing (Fig. 2) is stabilized by weak intermolecular C–H···O hydrogen bonds: the first one between a benzene H atom and the furan O atom (Table 1, C6–H6···O1$^{i}$), and the second one between a methyl H atom and the oxygen of the O═S═O unit (Table 1, C10–H10A···O2$^{ii}$). The crystal packing (Fig. 2) is further stabilized by an intermolecular C–H···$\pi$ interaction between the 4-chlorophenyl H atom and the benzene ring (Table 1; C13–H13···Cg$^{iii}$, Cg is the centroid of the C2–C7 benzene ring).

### S2. Experimental

77% 3-chloroperoxybenzoic acid (269 mg, 1.2 mmol) was added in small portions to a stirred solution of 3-(4-chlorophenylsulfanyl)-2,5-dimethyl-1-benzofuran (346 mg, 1.2 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 6h, 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 81%, m.p. 428-429 K; $R_f$ = 0.59 (benzene)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in acetone 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) = 1.2$U_{eq}$(C) for aryl and 1.5$U_{eq}$(C) for methyl H atoms.

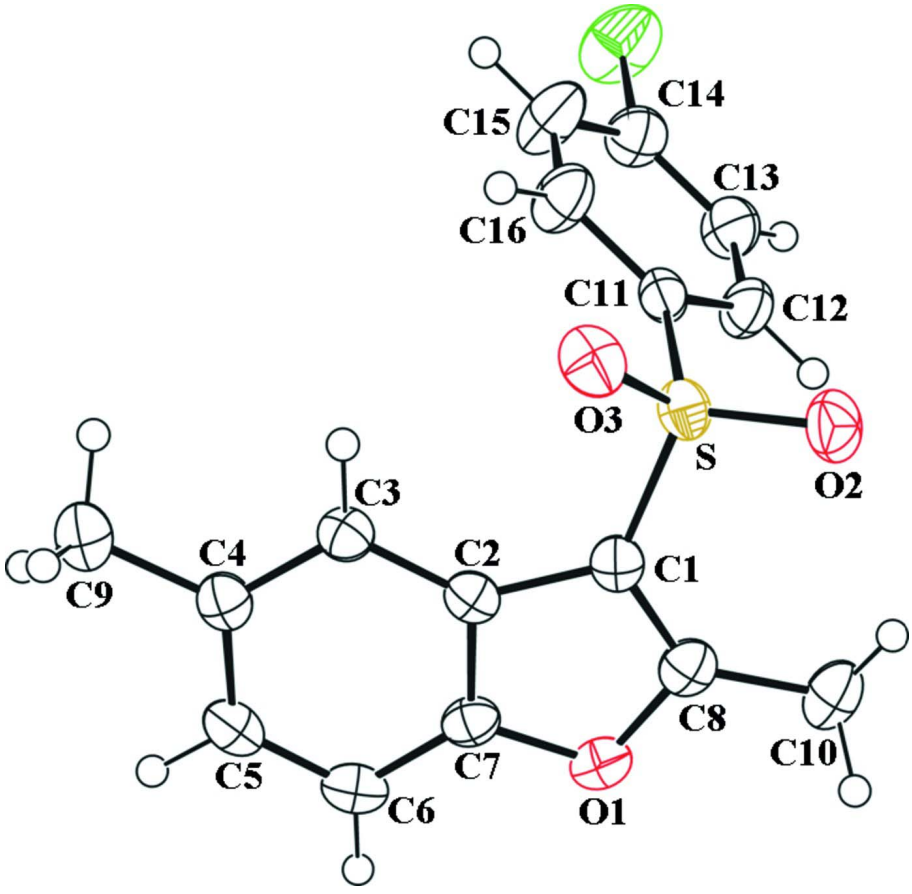


**Figure 1**

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.

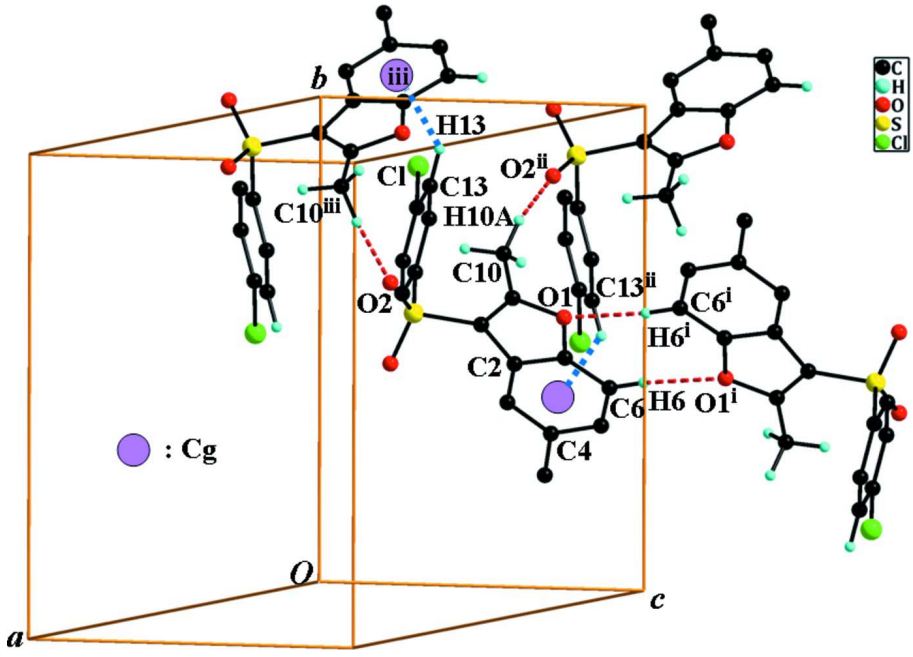


**Figure 2**

A view of the C–H···O and C–H···$\pi$ interactions (dotted lines) in the crystal structure of the title compound. Cg denotes the centroid of the C2-C7 benzene ring. [Symmetry codes: (i) - $x$, - $y$ + 1, - $z$ + 2; (ii) $x$, - $y$ +3/2, $z$ + 1/2; (iii) $x$, - $y$ + 3/2, $z$ - 1/2.]

### 3-(4-Chlorophenylsulfonyl)-2,5-dimethyl-1-benzofuran

*Crystal data*

$C_{16}H_{13}ClO_3S$
$M_r$ = 320.77
Monoclinic, $P2_1/c$
Hall symbol: -P_2ybc
$a$ = 15.3529 (3) Å
$b$ = 12.1495 (2) Å
$c$ = 8.2663 (2) Å
$\beta$ = 105.363 (1)°
$V$ = 1486.82 (5) Å$^3$
$Z$ = 4
$F(000)$ = 664
$D_x$ = 1.433 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4847 reflections
$\theta$ = 2.8–27.5°
$\mu$ = 0.40 mm$^{-1}$
$T$ = 177 K
Block, colourless
0.37 × 0.23 × 0.10 mm

*Data collection*

Bruker SMART APEXII CCD diffractometer
Radiation source: rotating anode
Graphite multilayer monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.867, $T_{max}$ = 0.962
13864 measured reflections
3398 independent reflections
2655 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 1.4°
$h$ = −19→19
$k$ = −15→14
$l$ = −10→10

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.107$
$S = 1.06$
3398 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
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.4243P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å$^{-3}$
$\Delta\rho_{min} = -0.34$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl | 0.48342 (4) | 0.92660 (5) | 0.73305 (10) | 0.0705 (2) |
| S | 0.17974 (3) | 0.58289 (4) | 0.44925 (5) | 0.03028 (14) |
| O1 | 0.04560 (8) | 0.56425 (10) | 0.79164 (16) | 0.0336 (3) |
| O2 | 0.11294 (8) | 0.63535 (12) | 0.31700 (15) | 0.0417 (3) |
| O3 | 0.22166 (9) | 0.48321 (11) | 0.41515 (15) | 0.0384 (3) |
| C1 | 0.13384 (11) | 0.55688 (14) | 0.6156 (2) | 0.0282 (4) |
| C2 | 0.17212 (10) | 0.48293 (14) | 0.75339 (19) | 0.0265 (4) |
| C3 | 0.24701 (11) | 0.41325 (14) | 0.7986 (2) | 0.0286 (4) |
| H3 | 0.2872 | 0.4070 | 0.7293 | 0.034* |
| C4 | 0.26171 (11) | 0.35337 (15) | 0.9461 (2) | 0.0305 (4) |
| C5 | 0.20127 (12) | 0.36427 (16) | 1.0465 (2) | 0.0336 (4) |
| H5 | 0.2120 | 0.3226 | 1.1471 | 0.040* |
| C6 | 0.12720 (12) | 0.43281 (15) | 1.0054 (2) | 0.0346 (4) |
| H6 | 0.0871 | 0.4400 | 1.0748 | 0.041* |
| C7 | 0.11476 (11) | 0.49046 (15) | 0.8570 (2) | 0.0287 (4) |
| C8 | 0.05880 (11) | 0.60332 (15) | 0.6451 (2) | 0.0312 (4) |
| C9 | 0.34169 (13) | 0.27807 (18) | 0.9993 (2) | 0.0426 (5) |
| H9A | 0.3251 | 0.2045 | 0.9527 | 0.064* |
| H9B | 0.3608 | 0.2738 | 1.1220 | 0.064* |
| H9C | 0.3914 | 0.3068 | 0.9579 | 0.064* |
| C10 | −0.00891 (12) | 0.68520 (16) | 0.5565 (3) | 0.0403 (5) |
| H10A | 0.0030 | 0.7562 | 0.6145 | 0.060* |
| H10B | −0.0696 | 0.6598 | 0.5558 | 0.060* |
| H10C | −0.0048 | 0.6936 | 0.4409 | 0.060* |
| C11 | 0.26643 (11) | 0.67929 (14) | 0.5303 (2) | 0.0285 (4) |

| | | | | |
|---|---|---|---|---|
| C12 | 0.24350 (12) | 0.78759 (16) | 0.5522 (2) | 0.0372 (4) |
| H12 | 0.1818 | 0.8092 | 0.5243 | 0.045* |
| C13 | 0.31025 (13) | 0.86365 (16) | 0.6145 (3) | 0.0409 (5) |
| H13 | 0.2954 | 0.9381 | 0.6301 | 0.049* |
| C14 | 0.39885 (13) | 0.83017 (17) | 0.6538 (3) | 0.0418 (5) |
| C15 | 0.42284 (13) | 0.72285 (18) | 0.6332 (3) | 0.0527 (6) |
| H15 | 0.4846 | 0.7016 | 0.6616 | 0.063* |
| C16 | 0.35555 (12) | 0.64652 (17) | 0.5705 (3) | 0.0435 (5) |
| H16 | 0.3706 | 0.5721 | 0.5552 | 0.052* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl | 0.0463 (3) | 0.0523 (4) | 0.1062 (6) | −0.0155 (3) | 0.0085 (3) | −0.0142 (3) |
| S | 0.0351 (2) | 0.0300 (3) | 0.0243 (2) | 0.00103 (18) | 0.00535 (17) | 0.00088 (17) |
| O1 | 0.0275 (6) | 0.0353 (7) | 0.0396 (7) | −0.0011 (5) | 0.0114 (5) | −0.0041 (6) |
| O2 | 0.0411 (7) | 0.0475 (9) | 0.0302 (7) | 0.0000 (6) | −0.0013 (5) | 0.0064 (6) |
| O3 | 0.0524 (8) | 0.0333 (7) | 0.0313 (6) | 0.0023 (6) | 0.0143 (6) | −0.0041 (6) |
| C1 | 0.0294 (8) | 0.0253 (9) | 0.0285 (8) | −0.0018 (7) | 0.0050 (7) | −0.0015 (7) |
| C2 | 0.0294 (8) | 0.0247 (9) | 0.0251 (8) | −0.0053 (7) | 0.0066 (6) | −0.0032 (7) |
| C3 | 0.0312 (8) | 0.0280 (9) | 0.0281 (8) | 0.0004 (7) | 0.0105 (7) | −0.0024 (7) |
| C4 | 0.0328 (9) | 0.0276 (9) | 0.0294 (8) | −0.0032 (7) | 0.0050 (7) | −0.0005 (7) |
| C5 | 0.0402 (10) | 0.0331 (10) | 0.0276 (8) | −0.0092 (8) | 0.0090 (7) | 0.0012 (8) |
| C6 | 0.0358 (9) | 0.0377 (11) | 0.0340 (9) | −0.0083 (8) | 0.0160 (8) | −0.0043 (8) |
| C7 | 0.0254 (8) | 0.0279 (9) | 0.0333 (9) | −0.0036 (7) | 0.0086 (7) | −0.0050 (7) |
| C8 | 0.0288 (8) | 0.0283 (9) | 0.0338 (9) | −0.0042 (7) | 0.0039 (7) | −0.0053 (8) |
| C9 | 0.0444 (11) | 0.0420 (12) | 0.0403 (10) | 0.0056 (9) | 0.0092 (9) | 0.0095 (9) |
| C10 | 0.0325 (9) | 0.0334 (11) | 0.0498 (11) | 0.0038 (8) | 0.0016 (8) | −0.0051 (9) |
| C11 | 0.0325 (8) | 0.0277 (9) | 0.0254 (8) | 0.0027 (7) | 0.0076 (7) | 0.0041 (7) |
| C12 | 0.0316 (9) | 0.0315 (10) | 0.0471 (11) | 0.0065 (8) | 0.0082 (8) | 0.0035 (9) |
| C13 | 0.0429 (10) | 0.0281 (10) | 0.0522 (12) | 0.0023 (8) | 0.0134 (9) | 0.0013 (9) |
| C14 | 0.0361 (10) | 0.0380 (11) | 0.0490 (11) | −0.0068 (8) | 0.0074 (8) | −0.0018 (9) |
| C15 | 0.0299 (10) | 0.0440 (13) | 0.0790 (16) | 0.0052 (9) | 0.0055 (10) | −0.0068 (12) |
| C16 | 0.0358 (10) | 0.0337 (11) | 0.0591 (13) | 0.0073 (8) | 0.0092 (9) | −0.0028 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl—C14 | 1.743 (2) | C6—H6 | 0.9500 |
| S—O3 | 1.4339 (14) | C8—C10 | 1.484 (2) |
| S—O2 | 1.4350 (13) | C9—H9A | 0.9800 |
| S—C1 | 1.7319 (17) | C9—H9B | 0.9800 |
| S—C11 | 1.7664 (18) | C9—H9C | 0.9800 |
| O1—C8 | 1.366 (2) | C10—H10A | 0.9800 |
| O1—C7 | 1.385 (2) | C10—H10B | 0.9800 |
| C1—C8 | 1.362 (2) | C10—H10C | 0.9800 |
| C1—C2 | 1.448 (2) | C11—C16 | 1.378 (2) |
| C2—C7 | 1.384 (2) | C11—C12 | 1.386 (3) |
| C2—C3 | 1.397 (2) | C12—C13 | 1.375 (3) |

| | | | |
|---|---|---|---|
| C3—C4 | 1.386 (2) | C12—H12 | 0.9500 |
| C3—H3 | 0.9500 | C13—C14 | 1.374 (3) |
| C4—C5 | 1.406 (2) | C13—H13 | 0.9500 |
| C4—C9 | 1.501 (2) | C14—C15 | 1.378 (3) |
| C5—C6 | 1.377 (3) | C15—C16 | 1.383 (3) |
| C5—H5 | 0.9500 | C15—H15 | 0.9500 |
| C6—C7 | 1.381 (3) | C16—H16 | 0.9500 |

| | | | |
|---|---|---|---|
| O3—S—O2 | 119.53 (8) | C4—C9—H9A | 109.5 |
| O3—S—C1 | 107.47 (8) | C4—C9—H9B | 109.5 |
| O2—S—C1 | 109.07 (8) | H9A—C9—H9B | 109.5 |
| O3—S—C11 | 107.60 (8) | C4—C9—H9C | 109.5 |
| O2—S—C11 | 108.01 (8) | H9A—C9—H9C | 109.5 |
| C1—S—C11 | 104.12 (8) | H9B—C9—H9C | 109.5 |
| C8—O1—C7 | 107.00 (13) | C8—C10—H10A | 109.5 |
| C8—C1—C2 | 107.60 (15) | C8—C10—H10B | 109.5 |
| C8—C1—S | 127.45 (14) | H10A—C10—H10B | 109.5 |
| C2—C1—S | 124.91 (13) | C8—C10—H10C | 109.5 |
| C7—C2—C3 | 119.21 (15) | H10A—C10—H10C | 109.5 |
| C7—C2—C1 | 104.70 (15) | H10B—C10—H10C | 109.5 |
| C3—C2—C1 | 136.09 (15) | C16—C11—C12 | 120.86 (17) |
| C4—C3—C2 | 118.96 (15) | C16—C11—S | 119.99 (14) |
| C4—C3—H3 | 120.5 | C12—C11—S | 119.15 (13) |
| C2—C3—H3 | 120.5 | C13—C12—C11 | 119.80 (17) |
| C3—C4—C5 | 119.40 (16) | C13—C12—H12 | 120.1 |
| C3—C4—C9 | 120.51 (16) | C11—C12—H12 | 120.1 |
| C5—C4—C9 | 120.09 (16) | C14—C13—C12 | 118.87 (18) |
| C6—C5—C4 | 122.84 (16) | C14—C13—H13 | 120.6 |
| C6—C5—H5 | 118.6 | C12—C13—H13 | 120.6 |
| C4—C5—H5 | 118.6 | C13—C14—C15 | 122.10 (18) |
| C5—C6—C7 | 115.89 (16) | C13—C14—Cl | 118.84 (16) |
| C5—C6—H6 | 122.1 | C15—C14—Cl | 119.06 (15) |
| C7—C6—H6 | 122.1 | C14—C15—C16 | 118.91 (18) |
| C6—C7—C2 | 123.71 (16) | C14—C15—H15 | 120.5 |
| C6—C7—O1 | 125.86 (15) | C16—C15—H15 | 120.5 |
| C2—C7—O1 | 110.43 (15) | C11—C16—C15 | 119.46 (18) |
| C1—C8—O1 | 110.27 (15) | C11—C16—H16 | 120.3 |
| C1—C8—C10 | 134.82 (17) | C15—C16—H16 | 120.3 |
| O1—C8—C10 | 114.91 (15) | | |

| | | | |
|---|---|---|---|
| O3—S—C1—C8 | −148.80 (16) | C8—O1—C7—C2 | 0.37 (18) |
| O2—S—C1—C8 | −17.84 (19) | C2—C1—C8—O1 | −0.30 (19) |
| C11—S—C1—C8 | 97.26 (17) | S—C1—C8—O1 | −178.16 (12) |
| O3—S—C1—C2 | 33.69 (16) | C2—C1—C8—C10 | 178.95 (18) |
| O2—S—C1—C2 | 164.64 (14) | S—C1—C8—C10 | 1.1 (3) |
| C11—S—C1—C2 | −80.26 (15) | C7—O1—C8—C1 | −0.03 (18) |
| C8—C1—C2—C7 | 0.51 (18) | C7—O1—C8—C10 | −179.45 (14) |
| S—C1—C2—C7 | 178.44 (13) | O3—S—C11—C16 | −8.62 (18) |

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| C8—C1—C2—C3 | −179.35 (18) | O2—S—C11—C16 | −138.91 (15) |
| S—C1—C2—C3 | −1.4 (3) | C1—S—C11—C16 | 105.24 (16) |
| C7—C2—C3—C4 | 0.1 (2) | O3—S—C11—C12 | 171.21 (14) |
| C1—C2—C3—C4 | 179.94 (18) | O2—S—C11—C12 | 40.92 (17) |
| C2—C3—C4—C5 | −0.1 (2) | C1—S—C11—C12 | −74.93 (16) |
| C2—C3—C4—C9 | −179.70 (16) | C16—C11—C12—C13 | 0.1 (3) |
| C3—C4—C5—C6 | −0.2 (3) | S—C11—C12—C13 | −179.71 (14) |
| C9—C4—C5—C6 | 179.34 (17) | C11—C12—C13—C14 | 0.0 (3) |
| C4—C5—C6—C7 | 0.6 (3) | C12—C13—C14—C15 | −0.2 (3) |
| C5—C6—C7—C2 | −0.6 (3) | C12—C13—C14—Cl | −179.91 (15) |
| C5—C6—C7—O1 | −179.53 (16) | C13—C14—C15—C16 | 0.2 (4) |
| C3—C2—C7—C6 | 0.3 (3) | Cl—C14—C15—C16 | 179.91 (18) |
| C1—C2—C7—C6 | −179.60 (16) | C12—C11—C16—C15 | −0.1 (3) |
| C3—C2—C7—O1 | 179.35 (14) | S—C11—C16—C15 | 179.72 (17) |
| C1—C2—C7—O1 | −0.54 (18) | C14—C15—C16—C11 | 0.0 (3) |
| C8—O1—C7—C6 | 179.41 (17) | | |

*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···O1$^{i}$ | 0.95 | 2.56 | 3.495 (2) | 167 |
| C10—H10*A*···O2$^{ii}$ | 0.98 | 2.43 | 3.279 (2) | 145 |
| C13—H13···*Cg*$^{iii}$ | 0.95 | 2.74 | 3.411 (2) | 128 |

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