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# 3-(3-Chlorophenylsulfinyl)-2,4,6,7-tetramethyl-1-benzofuran

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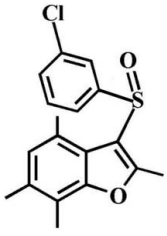
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.035; $wR$ factor = 0.099; data-to-parameter ratio = 19.2.

In the title compound, $C_{18}H_{17}ClO_2S$, the 3-chlorophenyl ring makes a dihedral angle of 72.62 (4)° with the mean plane of the benzofuran fragment. In the crystal, molecules are linked by weak intermolecular C—H···O and C—H···$\pi$ interactions. The crystal structure also exhibits a slipped $\pi$–$\pi$ interaction between the 3-chlorophenyl rings of adjacent molecules [centroid–centroid distance = 3.751 (2) Å, interplanar distance = 3.450 (2) Å and slippage = 1.472 (2) Å].

## Related literature

For the pharmacological activity of benzofuran compounds, see: Aslam *et al.* (2009); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For the crystal structures of related compounds, see: Choi *et al.* (2010, 2011).




## Experimental

### Crystal data

$C_{18}H_{17}ClO_2S$
$M_r$ = 332.83
Triclinic, $P\overline{1}$
$a$ = 7.4198 (1) Å
$b$ = 7.9792 (1) Å
$c$ = 14.5014 (2) Å
$\alpha$ = 105.965 (1)°
$\beta$ = 95.732 (1)°
$\gamma$ = 103.965 (1)°
$V$ = 788.21 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.38 mm$^{-1}$
$T$ = 173 K
0.26 × 0.25 × 0.25 mm

### Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.908, $T_{max}$ = 0.911
14786 measured reflections
3897 independent reflections
3622 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
$S$ = 0.95
3897 reflections
203 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

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

*Cg*1 is the centroid of the C2–C7 benzene ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C11—H11$B$···O2$^{i}$ | 0.98 | 2.60 | 3.5786 (16) | 175 |
| C12—H12$A$···O2$^{ii}$ | 0.98 | 2.40 | 3.3159 (17) | 155 |
| C10—H10$C$···$Cg1^{iii}$ | 0.98 | 2.79 | 3.615 (16) | 142 |

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

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: DS2170).

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# supporting information

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## 3-(3-Chlorophenylsulfinyl)-2,4,6,7-tetramethyl-1-benzofuran

**Hong Dae Choi, Pil Ja Seo and Uk Lee**

### S1. Comment

Substituted benzofuran analogues have drawn much attention owing to their valuable 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). These benzofuran derivatives occur in a wide range of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our continuing study of 2,4,6,7-tetramethyl-1-benzofuran derivatives containing either 3-(4-chlorophenylsulfinyl) (Choi *et al.*, 2010) or 3-(3-fluorophenylsulfinyl) (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 0.018 (1) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle between the 3-chlorophenyl ring and the mean plane of the benzofurn fragment is 72.62 (4)°. The crystal packing (Fig. 2) is stabilized by weak intermolecular C–H···O and C–H···$\pi$ interactions (Table 1, Cg1 is the centroid of the C2-C7 benzene ring). The crystal packing (Fig. 2) is further stabilized by a weak slipped $\pi$–$\pi$ interaction between the 3-chlorophenyl rings of adjacent molecules, with a Cg2···Cg2$^{iv}$ distance of 3.751 (2) Å and an interplanar distance of 3.450 (2) Å resulting in a slippage of 1.472 (2) Å (Cg2 is the centroid of the C13-C18 3-chlorophenyl ring).

### S2. Experimental

77% 3-chloroperoxybenzoic acid (224 mg, 1.0 mmol) was added in small portions to a stirred solution of 3-(3-chlorophenylsulfanyl)-2,4,6,7-tetramethyl-1-benzofuran (285 mg, 0.9 mmol) in dichloromethane (30 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 (hexane-ethyl acetate, 4:1 v/v) to afford the title compound as a colorless solid [yield 76%, m.p. 447-448 K; Rf = 0.52 (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 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.

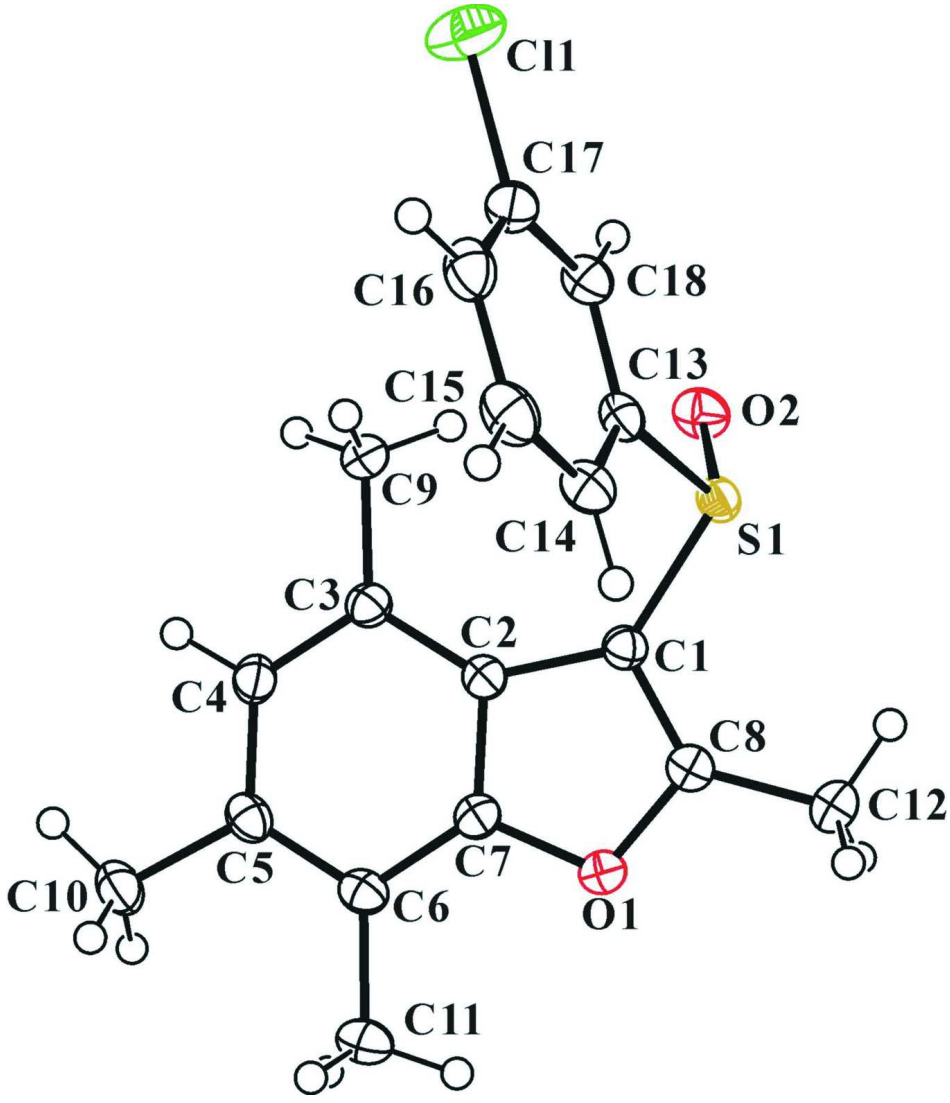


**Figure 1**

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 small spheres of arbitrary radius.

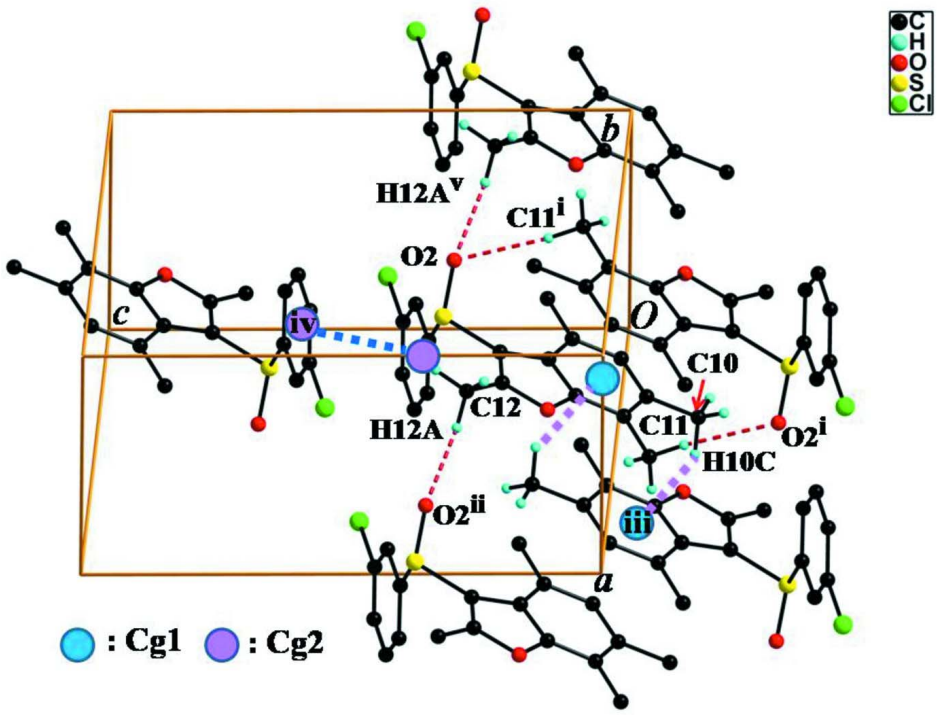


**Figure 2**

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

### 3-(3-Chlorophenylsulfinyl)-2,4,6,7-tetramethyl-1-benzofuran

*Crystal data*

$C_{18}H_{17}ClO_2S$
$M_r$ = 332.83
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 7.4198 (1) Å
$b$ = 7.9792 (1) Å
$c$ = 14.5014 (2) Å
$\alpha$ = 105.965 (1)°
$\beta$ = 95.732 (1)°
$\gamma$ = 103.965 (1)°
$V$ = 788.21 (2) Å$^3$
$Z$ = 2
$F$(000) = 348
$D_x$ = 1.402 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9057 reflections
$\theta$ = 2.7–28.3°
$\mu$ = 0.38 mm$^{-1}$
$T$ = 173 K
Block, colourless
0.26 × 0.25 × 0.25 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)
$T_{min}$ = 0.908, $T_{max}$ = 0.911
14786 measured reflections
3897 independent reflections
3622 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025
$\theta_{max}$ = 28.3°, $\theta_{min}$ = 1.5°
$h$ = −9→9
$k$ = −10→10
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.099$
$S = 0.95$
3897 reflections
203 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
$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 0.3249P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.36$ e Å$^{-3}$
$\Delta\rho_{min} = -0.39$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.53130 (4) | 0.65049 (4) | 0.33172 (2) | 0.02082 (9) |
| Cl1 | −0.00317 (6) | 0.23558 (6) | 0.46616 (3) | 0.04572 (13) |
| O1 | 0.79660 (12) | 0.52179 (12) | 0.11618 (6) | 0.02335 (19) |
| O2 | 0.36498 (14) | 0.72242 (13) | 0.32004 (7) | 0.0282 (2) |
| C1 | 0.59030 (17) | 0.55512 (16) | 0.21874 (8) | 0.0202 (2) |
| C2 | 0.48969 (16) | 0.40937 (15) | 0.13006 (8) | 0.0191 (2) |
| C3 | 0.30551 (17) | 0.29506 (16) | 0.09430 (9) | 0.0212 (2) |
| C4 | 0.27547 (18) | 0.17027 (17) | 0.00165 (9) | 0.0236 (2) |
| H4 | 0.1518 | 0.0915 | −0.0247 | 0.028* |
| C5 | 0.41627 (19) | 0.15371 (17) | −0.05513 (9) | 0.0232 (2) |
| C6 | 0.59915 (18) | 0.26984 (17) | −0.02096 (9) | 0.0220 (2) |
| C7 | 0.62560 (17) | 0.39462 (16) | 0.07062 (8) | 0.0204 (2) |
| C8 | 0.77070 (17) | 0.61729 (17) | 0.20508 (9) | 0.0227 (2) |
| C9 | 0.14666 (18) | 0.30115 (19) | 0.15074 (9) | 0.0270 (3) |
| H9A | 0.0265 | 0.2612 | 0.1053 | 0.040* |
| H9B | 0.1654 | 0.4257 | 0.1926 | 0.040* |
| H9C | 0.1445 | 0.2205 | 0.1911 | 0.040* |
| C10 | 0.3716 (2) | 0.00812 (19) | −0.15260 (9) | 0.0297 (3) |
| H10A | 0.4041 | 0.0640 | −0.2033 | 0.045* |
| H10B | 0.2366 | −0.0561 | −0.1674 | 0.045* |
| H10C | 0.4450 | −0.0781 | −0.1504 | 0.045* |
| C11 | 0.7563 (2) | 0.26059 (19) | −0.07831 (10) | 0.0285 (3) |
| H11A | 0.8681 | 0.3618 | −0.0442 | 0.043* |
| H11B | 0.7166 | 0.2685 | −0.1431 | 0.043* |
| H11C | 0.7866 | 0.1454 | −0.0850 | 0.043* |

| | | | | |
|---|---|---|---|---|
| C12 | 0.93714 (19) | 0.7651 (2) | 0.26499 (10) | 0.0317 (3) |
| H12A | 1.0409 | 0.7140 | 0.2781 | 0.048* |
| H12B | 0.9046 | 0.8265 | 0.3268 | 0.048* |
| H12C | 0.9761 | 0.8526 | 0.2298 | 0.048* |
| C13 | 0.44562 (18) | 0.44638 (16) | 0.36349 (8) | 0.0211 (2) |
| C14 | 0.55149 (19) | 0.32357 (18) | 0.35979 (9) | 0.0264 (3) |
| H14 | 0.6695 | 0.3438 | 0.3384 | 0.032* |
| C15 | 0.4822 (2) | 0.17083 (18) | 0.38788 (10) | 0.0305 (3) |
| H15 | 0.5528 | 0.0854 | 0.3851 | 0.037* |
| C16 | 0.3106 (2) | 0.14177 (18) | 0.42004 (10) | 0.0298 (3) |
| H16 | 0.2625 | 0.0365 | 0.4385 | 0.036* |
| C17 | 0.21090 (19) | 0.26868 (19) | 0.42478 (9) | 0.0276 (3) |
| C18 | 0.27641 (18) | 0.42257 (18) | 0.39725 (9) | 0.0246 (3) |
| H18 | 0.2069 | 0.5092 | 0.4015 | 0.030* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.02414 (16) | 0.01806 (15) | 0.01927 (15) | 0.00564 (11) | 0.00480 (11) | 0.00411 (11) |
| Cl1 | 0.0391 (2) | 0.0496 (2) | 0.0587 (3) | 0.01101 (18) | 0.02486 (18) | 0.0286 (2) |
| O1 | 0.0202 (4) | 0.0255 (4) | 0.0230 (4) | 0.0046 (3) | 0.0058 (3) | 0.0062 (3) |
| O2 | 0.0326 (5) | 0.0247 (5) | 0.0331 (5) | 0.0151 (4) | 0.0106 (4) | 0.0104 (4) |
| C1 | 0.0211 (5) | 0.0205 (5) | 0.0193 (5) | 0.0056 (4) | 0.0043 (4) | 0.0063 (4) |
| C2 | 0.0224 (6) | 0.0177 (5) | 0.0187 (5) | 0.0062 (4) | 0.0044 (4) | 0.0074 (4) |
| C3 | 0.0224 (6) | 0.0204 (5) | 0.0217 (5) | 0.0056 (4) | 0.0054 (4) | 0.0080 (4) |
| C4 | 0.0243 (6) | 0.0204 (6) | 0.0228 (6) | 0.0022 (5) | 0.0025 (4) | 0.0055 (5) |
| C5 | 0.0306 (6) | 0.0207 (6) | 0.0190 (5) | 0.0080 (5) | 0.0049 (4) | 0.0064 (4) |
| C6 | 0.0274 (6) | 0.0222 (6) | 0.0205 (5) | 0.0093 (5) | 0.0077 (4) | 0.0096 (4) |
| C7 | 0.0207 (5) | 0.0205 (5) | 0.0214 (5) | 0.0057 (4) | 0.0040 (4) | 0.0087 (4) |
| C8 | 0.0232 (6) | 0.0231 (6) | 0.0220 (5) | 0.0069 (5) | 0.0046 (4) | 0.0068 (5) |
| C9 | 0.0215 (6) | 0.0293 (6) | 0.0255 (6) | 0.0021 (5) | 0.0064 (5) | 0.0046 (5) |
| C10 | 0.0387 (7) | 0.0249 (6) | 0.0219 (6) | 0.0073 (5) | 0.0064 (5) | 0.0027 (5) |
| C11 | 0.0311 (7) | 0.0330 (7) | 0.0247 (6) | 0.0115 (5) | 0.0118 (5) | 0.0097 (5) |
| C12 | 0.0217 (6) | 0.0333 (7) | 0.0315 (7) | 0.0010 (5) | 0.0034 (5) | 0.0027 (6) |
| C13 | 0.0265 (6) | 0.0195 (5) | 0.0163 (5) | 0.0066 (4) | 0.0034 (4) | 0.0039 (4) |
| C14 | 0.0307 (6) | 0.0254 (6) | 0.0246 (6) | 0.0113 (5) | 0.0069 (5) | 0.0066 (5) |
| C15 | 0.0421 (8) | 0.0235 (6) | 0.0288 (6) | 0.0147 (6) | 0.0068 (6) | 0.0075 (5) |
| C16 | 0.0403 (7) | 0.0216 (6) | 0.0247 (6) | 0.0040 (5) | 0.0042 (5) | 0.0075 (5) |
| C17 | 0.0294 (6) | 0.0285 (6) | 0.0228 (6) | 0.0036 (5) | 0.0064 (5) | 0.0078 (5) |
| C18 | 0.0282 (6) | 0.0258 (6) | 0.0207 (6) | 0.0088 (5) | 0.0057 (5) | 0.0070 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O2 | 1.4949 (9) | C9—H9C | 0.9800 |
| S1—C1 | 1.7531 (12) | C10—H10A | 0.9800 |
| S1—C13 | 1.8001 (13) | C10—H10B | 0.9800 |
| Cl1—C17 | 1.7401 (14) | C10—H10C | 0.9800 |
| O1—C8 | 1.3635 (14) | C11—H11A | 0.9800 |

| | | | |
|---|---|---|---|
| O1—C7 | 1.3851 (14) | C11—H11B | 0.9800 |
| C1—C8 | 1.3651 (17) | C11—H11C | 0.9800 |
| C1—C2 | 1.4594 (16) | C12—H12A | 0.9800 |
| C2—C7 | 1.3960 (16) | C12—H12B | 0.9800 |
| C2—C3 | 1.4018 (17) | C12—H12C | 0.9800 |
| C3—C4 | 1.3941 (17) | C13—C18 | 1.3823 (17) |
| C3—C9 | 1.5032 (16) | C13—C14 | 1.3897 (17) |
| C4—C5 | 1.4020 (17) | C14—C15 | 1.3886 (19) |
| C4—H4 | 0.9500 | C14—H14 | 0.9500 |
| C5—C6 | 1.3970 (18) | C15—C16 | 1.388 (2) |
| C5—C10 | 1.5081 (17) | C15—H15 | 0.9500 |
| C6—C7 | 1.3856 (17) | C16—C17 | 1.382 (2) |
| C6—C11 | 1.5025 (17) | C16—H16 | 0.9500 |
| C8—C12 | 1.4797 (18) | C17—C18 | 1.3870 (19) |
| C9—H9A | 0.9800 | C18—H18 | 0.9500 |
| C9—H9B | 0.9800 | | |

| | | | |
|---|---|---|---|
| O2—S1—C1 | 111.44 (6) | C5—C10—H10B | 109.5 |
| O2—S1—C13 | 105.69 (6) | H10A—C10—H10B | 109.5 |
| C1—S1—C13 | 99.12 (5) | C5—C10—H10C | 109.5 |
| C8—O1—C7 | 106.80 (9) | H10A—C10—H10C | 109.5 |
| C8—C1—C2 | 107.14 (10) | H10B—C10—H10C | 109.5 |
| C8—C1—S1 | 118.34 (9) | C6—C11—H11A | 109.5 |
| C2—C1—S1 | 134.45 (9) | C6—C11—H11B | 109.5 |
| C7—C2—C3 | 118.68 (11) | H11A—C11—H11B | 109.5 |
| C7—C2—C1 | 104.27 (10) | C6—C11—H11C | 109.5 |
| C3—C2—C1 | 137.04 (11) | H11A—C11—H11C | 109.5 |
| C4—C3—C2 | 116.04 (11) | H11B—C11—H11C | 109.5 |
| C4—C3—C9 | 120.50 (11) | C8—C12—H12A | 109.5 |
| C2—C3—C9 | 123.45 (11) | C8—C12—H12B | 109.5 |
| C3—C4—C5 | 124.13 (12) | H12A—C12—H12B | 109.5 |
| C3—C4—H4 | 117.9 | C8—C12—H12C | 109.5 |
| C5—C4—H4 | 117.9 | H12A—C12—H12C | 109.5 |
| C6—C5—C4 | 120.18 (11) | H12B—C12—H12C | 109.5 |
| C6—C5—C10 | 119.76 (11) | C18—C13—C14 | 121.49 (12) |
| C4—C5—C10 | 120.05 (12) | C18—C13—S1 | 117.34 (9) |
| C7—C6—C5 | 114.84 (11) | C14—C13—S1 | 121.06 (10) |
| C7—C6—C11 | 122.20 (12) | C15—C14—C13 | 118.97 (12) |
| C5—C6—C11 | 122.96 (11) | C15—C14—H14 | 120.5 |
| O1—C7—C6 | 123.21 (11) | C13—C14—H14 | 120.5 |
| O1—C7—C2 | 110.72 (10) | C16—C15—C14 | 120.63 (12) |
| C6—C7—C2 | 126.06 (11) | C16—C15—H15 | 119.7 |
| O1—C8—C1 | 111.04 (11) | C14—C15—H15 | 119.7 |
| O1—C8—C12 | 115.43 (11) | C17—C16—C15 | 118.86 (13) |
| C1—C8—C12 | 133.53 (12) | C17—C16—H16 | 120.6 |
| C3—C9—H9A | 109.5 | C15—C16—H16 | 120.6 |
| C3—C9—H9B | 109.5 | C16—C17—C18 | 121.86 (13) |
| H9A—C9—H9B | 109.5 | C16—C17—Cl1 | 119.46 (11) |

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|---|---|---|---|
| C3—C9—H9C | 109.5 | C18—C17—Cl1 | 118.68 (11) |
| H9A—C9—H9C | 109.5 | C13—C18—C17 | 118.15 (12) |
| H9B—C9—H9C | 109.5 | C13—C18—H18 | 120.9 |
| C5—C10—H10A | 109.5 | C17—C18—H18 | 120.9 |
| | | | |
| O2—S1—C1—C8 | 125.23 (10) | C11—C6—C7—C2 | −178.00 (11) |
| C13—S1—C1—C8 | −123.83 (10) | C3—C2—C7—O1 | 177.83 (10) |
| O2—S1—C1—C2 | −58.15 (13) | C1—C2—C7—O1 | −1.15 (12) |
| C13—S1—C1—C2 | 52.78 (13) | C3—C2—C7—C6 | −3.17 (18) |
| C8—C1—C2—C7 | 1.49 (13) | C1—C2—C7—C6 | 177.85 (11) |
| S1—C1—C2—C7 | −175.39 (10) | C7—O1—C8—C1 | 0.63 (13) |
| C8—C1—C2—C3 | −177.20 (13) | C7—O1—C8—C12 | −178.36 (11) |
| S1—C1—C2—C3 | 5.9 (2) | C2—C1—C8—O1 | −1.34 (14) |
| C7—C2—C3—C4 | 1.96 (16) | S1—C1—C8—O1 | 176.13 (8) |
| C1—C2—C3—C4 | −179.49 (13) | C2—C1—C8—C12 | 177.39 (14) |
| C7—C2—C3—C9 | −178.71 (11) | S1—C1—C8—C12 | −5.1 (2) |
| C1—C2—C3—C9 | −0.2 (2) | O2—S1—C13—C18 | −17.61 (11) |
| C2—C3—C4—C5 | 0.39 (18) | C1—S1—C13—C18 | −133.06 (10) |
| C9—C3—C4—C5 | −178.96 (12) | O2—S1—C13—C14 | 166.23 (10) |
| C3—C4—C5—C6 | −1.86 (19) | C1—S1—C13—C14 | 50.79 (11) |
| C3—C4—C5—C10 | 177.04 (12) | C18—C13—C14—C15 | 2.02 (19) |
| C4—C5—C6—C7 | 0.82 (17) | S1—C13—C14—C15 | 178.01 (10) |
| C10—C5—C6—C7 | −178.09 (11) | C13—C14—C15—C16 | −0.6 (2) |
| C4—C5—C6—C11 | −179.50 (11) | C14—C15—C16—C17 | −0.8 (2) |
| C10—C5—C6—C11 | 1.59 (18) | C15—C16—C17—C18 | 0.8 (2) |
| C8—O1—C7—C6 | −178.65 (11) | C15—C16—C17—Cl1 | −179.31 (10) |
| C8—O1—C7—C2 | 0.39 (13) | C14—C13—C18—C17 | −2.01 (18) |
| C5—C6—C7—O1 | −179.43 (10) | S1—C13—C18—C17 | −178.15 (9) |
| C11—C6—C7—O1 | 0.88 (18) | C16—C17—C18—C13 | 0.59 (19) |
| C5—C6—C7—C2 | 1.68 (18) | Cl1—C17—C18—C13 | −179.31 (9) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C2–C7 benzene ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C11—H11*B*···O2$^{i}$ | 0.98 | 2.60 | 3.5786 (16) | 175 |
| C12—H12*A*···O2$^{ii}$ | 0.98 | 2.40 | 3.3159 (17) | 155 |
| C10—H10*C*···*Cg*1$^{iii}$ | 0.98 | 2.79 | 3.615 (16) | 142 |

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