

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

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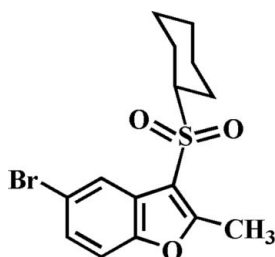
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.028; wR factor = 0.073; data-to-parameter ratio = 18.6.

In the title compound, $\text{C}_{15}\text{H}_{17}\text{BrO}_3\text{S}$, the cyclohexyl ring adopts a practically undistorted chair conformation [endocyclic torsion angles are within a 54.5 – 56.4 (3) $^\circ$ range] and the arylsulfonyl unit is positioned equatorial relative to the cyclohexyl group. In the crystal, molecules are linked through $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and donor–acceptor $\text{Br}\cdots\text{O}$ contacts [3.250 (2) Å]. The crystal structure also exhibits aromatic π – π overlap between the benzene and furan rings of neighbouring molecules [centroid–centroid distance = 3.635 (2) 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 structural studies of related 3-arylsulfonyl-5-bromo-2-methyl-1-benzofuran derivatives, see: Choi *et al.* (2008, 2010). For a review of halogen bonding, see: Politzer *et al.* (2007).



Experimental

Crystal data

| | |
|--|-------------------------------------|
| $\text{C}_{15}\text{H}_{17}\text{BrO}_3\text{S}$ | $\gamma = 96.385$ (1) $^\circ$ |
| $M_r = 357.26$ | $V = 731.95$ (2) Å ³ |
| Triclinic, $P\bar{1}$ | $Z = 2$ |
| $a = 6.3452$ (1) Å | Mo $K\alpha$ radiation |
| $b = 8.2065$ (1) Å | $\mu = 2.95$ mm ⁻¹ |
| $c = 14.4866$ (2) Å | $T = 173$ K |
| $\alpha = 98.842$ (1) $^\circ$ | $0.33 \times 0.26 \times 0.23$ mm |
| $\beta = 97.693$ (1) $^\circ$ | |

Data collection

| | |
|--|--|
| Bruker SMART APEXII CCD diffractometer | 13107 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2009) | 3377 independent reflections |
| $T_{\min} = 0.585$, $T_{\max} = 0.746$ | 3109 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.034$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.028$ | 182 parameters |
| $wR(F^2) = 0.073$ | H-atom parameters constrained |
| $S = 1.07$ | $\Delta\rho_{\text{max}} = 0.35$ e Å ⁻³ |
| 3377 reflections | $\Delta\rho_{\text{min}} = -0.70$ e Å ⁻³ |

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{C6}-\text{H6}\cdots\text{O1}^{\text{i}}$ | 0.95 | 2.57 | 3.518 (2) | 174 |
| $\text{C9}-\text{H9B}\cdots\text{O3}^{\text{ii}}$ | 0.98 | 2.55 | 3.303 (2) | 134 |

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

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.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2001).

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supplementary materials

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

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Comment

Many compounds containing a benzofuran ring show diverse 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-bromo-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 0.006 (2) Å from the least-squares plane defined by the nine constituent atoms. The cyclohexyl ring is in the chair form and arylsulfonyl moiety is positioned equatorial relative to the cyclohexyl group. The molecular packing (Fig. 2) is stabilized by intermolecular C—H \cdots O hydrogen bonds - between an arene H atom and the furan O atom (Table 1; C6—H6 \cdots O1ⁱ), and between a methyl H atom and a sulfonyl oxygen (Table 1; C9—H9B \cdots O3ⁱⁱ). The crystal structure is further stabilized by Br \cdots O halogen bonding between the bromine and an oxygen of the sulfonyl group [Br1 \cdots O3ⁱⁱⁱ = 3.250 (2) Å, C4—Br1 \cdots O3ⁱⁱⁱ = 165.29 (6)°] (Politzer *et al.*, 2007). The crystal packing (Fig. 2) also exhibits π - π overlap between the benzene and furan rings of neighbouring molecules, with a Cg1 \cdots Cg2^{iv} distance of 3.633 (2) Å (Cg1 and Cg2 are the centroids of the C2-C7 benzene ring and the C1/C2/C7/O1/C8 furan ring, respectively), wherein the inter-planar distance between the benzene and furan rings is 3.391 (2) Å.

Experimental

77% 3-chloroperoxybenzoic acid (381 mg, 1.7 mmol) was added in small portions to a stirred solution of 5-bromo-3-cyclohexylsulfonyl-2-methyl-1-benzofuran (260 mg, 0.8 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 5h, 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. 446–447 K; R_f = 0.58 (hexane-ethyl acetate, 4:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of acetone solution of the title compound at room temperature.

Refinement

All H atoms were positioned geometrically and refined using a riding and rotating 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, methylene and $1.5U_{eq}(C)$ for methyl H atoms.

Figures

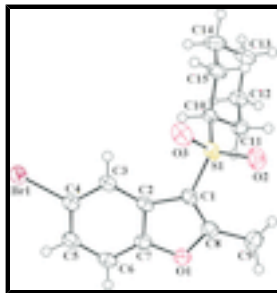


Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

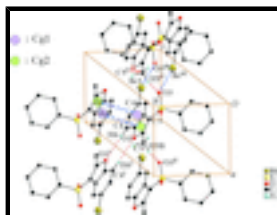


Fig. 2. A view of the C—H...O, Br...O and π - π interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) $-x + 2, -y + 2, -z + 1$; (ii) $x + 1, y, z$; (iii) $-x, -y + 1, -z + 1$; (iv) $-x + 1, -y + 2, -z + 1$; (v) $x - 1, y, z$.]

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

Crystal data

$C_{15}H_{17}BrO_3S$

$M_r = 357.26$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 6.3452\ (1)\ \text{\AA}$

$b = 8.2065\ (1)\ \text{\AA}$

$c = 14.4866\ (2)\ \text{\AA}$

$\alpha = 98.842\ (1)^\circ$

$\beta = 97.693\ (1)^\circ$

$\gamma = 96.385\ (1)^\circ$

$V = 731.95\ (2)\ \text{\AA}^3$

$Z = 2$

$F(000) = 364$

$D_x = 1.621\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 8112 reflections

$\theta = 2.7\text{--}27.5^\circ$

$\mu = 2.95\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Block, colourless

$0.33 \times 0.26 \times 0.23\ \text{mm}$

Data collection

Bruker SMART APEXII CCD diffractometer

3377 independent reflections

Radiation source: rotating anode graphite multilayer

3109 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

Detector resolution: $10.0\ \text{pixels mm}^{-1}$

$\theta_{\text{max}} = 27.6^\circ, \theta_{\text{min}} = 1.4^\circ$

φ and ω scans

$h = -8 \rightarrow 8$

Absorption correction: multi-scan (SADABS; Bruker, 2009)

$k = -10 \rightarrow 10$

$T_{\text{min}} = 0.585, T_{\text{max}} = 0.746$

$l = -18 \rightarrow 18$

13107 measured reflections

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.028$ | Hydrogen site location: difference Fourier map |
| $wR(F^2) = 0.073$ | H-atom parameters constrained |
| $S = 1.07$ | $w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.2624P]$ |
| 3377 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 182 parameters | $(\Delta/\sigma)_{\max} = 0.001$ |
| 0 restraints | $\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$ |
| | $\Delta\rho_{\min} = -0.70 \text{ e } \text{\AA}^{-3}$ |

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|---------------|----------------------------------|
| Br1 | 0.24178 (3) | 0.58796 (3) | 0.634104 (12) | 0.03547 (8) |
| S1 | 0.21139 (7) | 0.69361 (6) | 0.22168 (3) | 0.02801 (11) |
| O1 | 0.7467 (2) | 0.92120 (16) | 0.38017 (9) | 0.0310 (3) |
| O2 | 0.2068 (3) | 0.78049 (19) | 0.14233 (10) | 0.0400 (3) |
| O3 | 0.0254 (2) | 0.6830 (2) | 0.26875 (10) | 0.0396 (3) |
| C1 | 0.4294 (3) | 0.7824 (2) | 0.30762 (12) | 0.0267 (4) |
| C2 | 0.4500 (3) | 0.7619 (2) | 0.40566 (12) | 0.0261 (3) |
| C3 | 0.3234 (3) | 0.6829 (2) | 0.46111 (12) | 0.0284 (4) |
| H3 | 0.1862 | 0.6225 | 0.4355 | 0.034* |
| C4 | 0.4078 (3) | 0.6967 (2) | 0.55581 (13) | 0.0286 (4) |
| C5 | 0.6076 (3) | 0.7838 (3) | 0.59542 (13) | 0.0324 (4) |
| H5 | 0.6582 | 0.7887 | 0.6607 | 0.039* |
| C6 | 0.7337 (3) | 0.8635 (3) | 0.54056 (14) | 0.0330 (4) |
| H6 | 0.8706 | 0.9243 | 0.5663 | 0.040* |
| C7 | 0.6495 (3) | 0.8496 (2) | 0.44644 (13) | 0.0284 (4) |
| C8 | 0.6100 (3) | 0.8776 (2) | 0.29616 (13) | 0.0290 (4) |
| C9 | 0.6862 (4) | 0.9444 (3) | 0.21558 (15) | 0.0365 (4) |
| H9A | 0.5693 | 0.9244 | 0.1619 | 0.055* |
| H9B | 0.8070 | 0.8887 | 0.1974 | 0.055* |

supplementary materials

| | | | | |
|------|------------|------------|--------------|------------|
| H9C | 0.7330 | 1.0643 | 0.2340 | 0.055* |
| C10 | 0.2636 (3) | 0.4859 (2) | 0.18543 (12) | 0.0244 (3) |
| H10 | 0.3071 | 0.4386 | 0.2436 | 0.029* |
| C11 | 0.4467 (3) | 0.4811 (2) | 0.12705 (13) | 0.0288 (4) |
| H11A | 0.5802 | 0.5433 | 0.1657 | 0.035* |
| H11B | 0.4124 | 0.5353 | 0.0714 | 0.035* |
| C12 | 0.4807 (3) | 0.3011 (3) | 0.09420 (14) | 0.0328 (4) |
| H12A | 0.5919 | 0.2997 | 0.0523 | 0.039* |
| H12B | 0.5334 | 0.2522 | 0.1498 | 0.039* |
| C13 | 0.2750 (3) | 0.1955 (3) | 0.04136 (16) | 0.0419 (5) |
| H13A | 0.2310 | 0.2363 | -0.0182 | 0.050* |
| H13B | 0.3015 | 0.0787 | 0.0249 | 0.050* |
| C14 | 0.0960 (4) | 0.2023 (3) | 0.10074 (18) | 0.0474 (6) |
| H14A | 0.1341 | 0.1512 | 0.1573 | 0.057* |
| H14B | -0.0373 | 0.1371 | 0.0636 | 0.057* |
| C15 | 0.0563 (3) | 0.3812 (3) | 0.13187 (14) | 0.0358 (4) |
| H15A | -0.0560 | 0.3825 | 0.1732 | 0.043* |
| H15B | 0.0050 | 0.4294 | 0.0757 | 0.043* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Br1 | 0.03585 (12) | 0.04254 (13) | 0.02647 (11) | 0.00000 (9) | 0.00393 (8) | 0.00562 (8) |
| S1 | 0.0262 (2) | 0.0334 (2) | 0.0240 (2) | 0.00874 (18) | 0.00065 (16) | 0.00314 (18) |
| O1 | 0.0298 (7) | 0.0289 (7) | 0.0321 (7) | 0.0000 (6) | 0.0053 (5) | 0.0004 (5) |
| O2 | 0.0471 (8) | 0.0414 (8) | 0.0332 (7) | 0.0134 (7) | -0.0016 (6) | 0.0129 (6) |
| O3 | 0.0277 (7) | 0.0553 (10) | 0.0352 (7) | 0.0134 (7) | 0.0045 (6) | 0.0009 (7) |
| C1 | 0.0294 (9) | 0.0247 (9) | 0.0243 (8) | 0.0049 (7) | 0.0024 (7) | -0.0003 (7) |
| C2 | 0.0272 (8) | 0.0236 (8) | 0.0248 (8) | 0.0043 (7) | 0.0017 (6) | -0.0026 (7) |
| C3 | 0.0280 (9) | 0.0290 (9) | 0.0251 (8) | 0.0023 (7) | 0.0012 (7) | -0.0013 (7) |
| C4 | 0.0308 (9) | 0.0270 (9) | 0.0266 (8) | 0.0035 (7) | 0.0038 (7) | 0.0007 (7) |
| C5 | 0.0348 (10) | 0.0330 (10) | 0.0255 (8) | 0.0026 (8) | -0.0020 (7) | -0.0002 (7) |
| C6 | 0.0278 (9) | 0.0323 (10) | 0.0327 (10) | -0.0025 (8) | -0.0031 (7) | -0.0025 (8) |
| C7 | 0.0282 (9) | 0.0256 (9) | 0.0296 (9) | 0.0029 (7) | 0.0045 (7) | -0.0009 (7) |
| C8 | 0.0337 (9) | 0.0242 (9) | 0.0287 (9) | 0.0076 (7) | 0.0051 (7) | 0.0000 (7) |
| C9 | 0.0413 (11) | 0.0336 (10) | 0.0379 (10) | 0.0078 (9) | 0.0114 (9) | 0.0098 (8) |
| C10 | 0.0228 (8) | 0.0285 (9) | 0.0197 (7) | 0.0003 (7) | 0.0004 (6) | 0.0023 (6) |
| C11 | 0.0243 (8) | 0.0303 (9) | 0.0312 (9) | 0.0018 (7) | 0.0057 (7) | 0.0032 (7) |
| C12 | 0.0284 (9) | 0.0316 (10) | 0.0353 (10) | 0.0052 (8) | 0.0019 (7) | -0.0018 (8) |
| C13 | 0.0363 (11) | 0.0423 (12) | 0.0377 (11) | 0.0002 (9) | -0.0012 (9) | -0.0124 (9) |
| C14 | 0.0374 (11) | 0.0441 (13) | 0.0496 (13) | -0.0147 (10) | 0.0052 (10) | -0.0107 (10) |
| C15 | 0.0213 (8) | 0.0485 (12) | 0.0313 (9) | -0.0042 (8) | 0.0018 (7) | -0.0047 (9) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|---------------------|-------------|--------|--------|
| Br1—O3 ⁱ | 3.250 (2) | C9—H9A | 0.9800 |
| Br1—C4 | 1.901 (2) | C9—H9B | 0.9800 |
| S1—O3 | 1.4409 (15) | C9—H9C | 0.9800 |

| | | | |
|------------------------|-------------|---------------|-------------|
| S1—O2 | 1.4416 (15) | C10—C11 | 1.526 (2) |
| S1—C1 | 1.7408 (18) | C10—C15 | 1.530 (2) |
| S1—C10 | 1.7852 (18) | C10—H10 | 1.0000 |
| O1—C8 | 1.370 (2) | C11—C12 | 1.529 (3) |
| O1—C7 | 1.378 (2) | C11—H11A | 0.9900 |
| C1—C8 | 1.357 (3) | C11—H11B | 0.9900 |
| C1—C2 | 1.446 (2) | C12—C13 | 1.523 (3) |
| C2—C3 | 1.388 (3) | C12—H12A | 0.9900 |
| C2—C7 | 1.392 (3) | C12—H12B | 0.9900 |
| C3—C4 | 1.387 (2) | C13—C14 | 1.515 (3) |
| C3—H3 | 0.9500 | C13—H13A | 0.9900 |
| C4—C5 | 1.387 (3) | C13—H13B | 0.9900 |
| C5—C6 | 1.383 (3) | C14—C15 | 1.527 (3) |
| C5—H5 | 0.9500 | C14—H14A | 0.9900 |
| C6—C7 | 1.379 (3) | C14—H14B | 0.9900 |
| C6—H6 | 0.9500 | C15—H15A | 0.9900 |
| C8—C9 | 1.479 (3) | C15—H15B | 0.9900 |
| C4—Br1—O3 ⁱ | 165.29 (6) | H9B—C9—H9C | 109.5 |
| O3—S1—O2 | 118.38 (9) | C11—C10—C15 | 112.06 (14) |
| O3—S1—C1 | 106.84 (9) | C11—C10—S1 | 111.82 (13) |
| O2—S1—C1 | 109.77 (9) | C15—C10—S1 | 108.98 (13) |
| O3—S1—C10 | 107.26 (9) | C11—C10—H10 | 107.9 |
| O2—S1—C10 | 109.22 (9) | C15—C10—H10 | 107.9 |
| C1—S1—C10 | 104.45 (8) | S1—C10—H10 | 107.9 |
| C8—O1—C7 | 106.96 (14) | C10—C11—C12 | 110.24 (15) |
| C8—C1—C2 | 107.72 (16) | C10—C11—H11A | 109.6 |
| C8—C1—S1 | 127.65 (14) | C12—C11—H11A | 109.6 |
| C2—C1—S1 | 124.60 (14) | C10—C11—H11B | 109.6 |
| C3—C2—C7 | 119.65 (16) | C12—C11—H11B | 109.6 |
| C3—C2—C1 | 135.86 (17) | H11A—C11—H11B | 108.1 |
| C7—C2—C1 | 104.48 (16) | C13—C12—C11 | 111.97 (16) |
| C4—C3—C2 | 116.54 (17) | C13—C12—H12A | 109.2 |
| C4—C3—H3 | 121.7 | C11—C12—H12A | 109.2 |
| C2—C3—H3 | 121.7 | C13—C12—H12B | 109.2 |
| C3—C4—C5 | 123.20 (18) | C11—C12—H12B | 109.2 |
| C3—C4—Br1 | 118.01 (14) | H12A—C12—H12B | 107.9 |
| C5—C4—Br1 | 118.78 (14) | C14—C13—C12 | 111.09 (17) |
| C6—C5—C4 | 120.46 (17) | C14—C13—H13A | 109.4 |
| C6—C5—H5 | 119.8 | C12—C13—H13A | 109.4 |
| C4—C5—H5 | 119.8 | C14—C13—H13B | 109.4 |
| C7—C6—C5 | 116.23 (17) | C12—C13—H13B | 109.4 |
| C7—C6—H6 | 121.9 | H13A—C13—H13B | 108.0 |
| C5—C6—H6 | 121.9 | C13—C14—C15 | 111.34 (19) |
| O1—C7—C6 | 125.59 (17) | C13—C14—H14A | 109.4 |
| O1—C7—C2 | 110.49 (16) | C15—C14—H14A | 109.4 |
| C6—C7—C2 | 123.91 (18) | C13—C14—H14B | 109.4 |
| C1—C8—O1 | 110.33 (16) | C15—C14—H14B | 109.4 |
| C1—C8—C9 | 134.57 (18) | H14A—C14—H14B | 108.0 |

supplementary materials

| | | | |
|--------------|--------------|-----------------|--------------|
| O1—C8—C9 | 115.09 (17) | C14—C15—C10 | 110.09 (16) |
| C8—C9—H9A | 109.5 | C14—C15—H15A | 109.6 |
| C8—C9—H9B | 109.5 | C10—C15—H15A | 109.6 |
| H9A—C9—H9B | 109.5 | C14—C15—H15B | 109.6 |
| C8—C9—H9C | 109.5 | C10—C15—H15B | 109.6 |
| H9A—C9—H9C | 109.5 | H15A—C15—H15B | 108.2 |
| O3—S1—C1—C8 | -150.39 (17) | C3—C2—C7—C6 | 0.4 (3) |
| O2—S1—C1—C8 | -20.86 (19) | C1—C2—C7—C6 | 179.62 (18) |
| C10—S1—C1—C8 | 96.14 (18) | C2—C1—C8—O1 | -0.3 (2) |
| O3—S1—C1—C2 | 31.47 (18) | S1—C1—C8—O1 | -178.67 (13) |
| O2—S1—C1—C2 | 161.01 (15) | C2—C1—C8—C9 | -179.0 (2) |
| C10—S1—C1—C2 | -81.99 (16) | S1—C1—C8—C9 | 2.6 (3) |
| C8—C1—C2—C3 | 178.9 (2) | C7—O1—C8—C1 | 0.59 (19) |
| S1—C1—C2—C3 | -2.7 (3) | C7—O1—C8—C9 | 179.58 (15) |
| C8—C1—C2—C7 | -0.1 (2) | O3—S1—C10—C11 | 175.09 (12) |
| S1—C1—C2—C7 | 178.32 (13) | O2—S1—C10—C11 | 45.64 (14) |
| C7—C2—C3—C4 | -0.3 (3) | C1—S1—C10—C11 | -71.74 (14) |
| C1—C2—C3—C4 | -179.25 (19) | O3—S1—C10—C15 | 50.66 (14) |
| C2—C3—C4—C5 | -0.1 (3) | O2—S1—C10—C15 | -78.79 (14) |
| C2—C3—C4—Br1 | -179.16 (13) | C1—S1—C10—C15 | 163.83 (13) |
| C3—C4—C5—C6 | 0.4 (3) | C15—C10—C11—C12 | -55.1 (2) |
| Br1—C4—C5—C6 | 179.53 (15) | S1—C10—C11—C12 | -177.82 (12) |
| C4—C5—C6—C7 | -0.4 (3) | C10—C11—C12—C13 | 54.5 (2) |
| C8—O1—C7—C6 | -179.79 (18) | C11—C12—C13—C14 | -55.5 (3) |
| C8—O1—C7—C2 | -0.68 (19) | C12—C13—C14—C15 | 56.4 (3) |
| C5—C6—C7—O1 | 178.95 (17) | C13—C14—C15—C10 | -56.4 (2) |
| C5—C6—C7—C2 | 0.0 (3) | C11—C10—C15—C14 | 56.2 (2) |
| C3—C2—C7—O1 | -178.72 (15) | S1—C10—C15—C14 | -179.50 (15) |
| C1—C2—C7—O1 | 0.5 (2) | | |

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|-------|-------------|-------------|---------------|
| C6—H6 \cdots O1 ⁱⁱ | 0.95 | 2.57 | 3.518 (2) | 174 |
| C9—H9B \cdots O3 ⁱⁱⁱ | 0.98 | 2.55 | 3.303 (2) | 134 |

Symmetry codes: (ii) $-x+2, -y+2, -z+1$; (iii) $x+1, y, z$.

Fig. 1

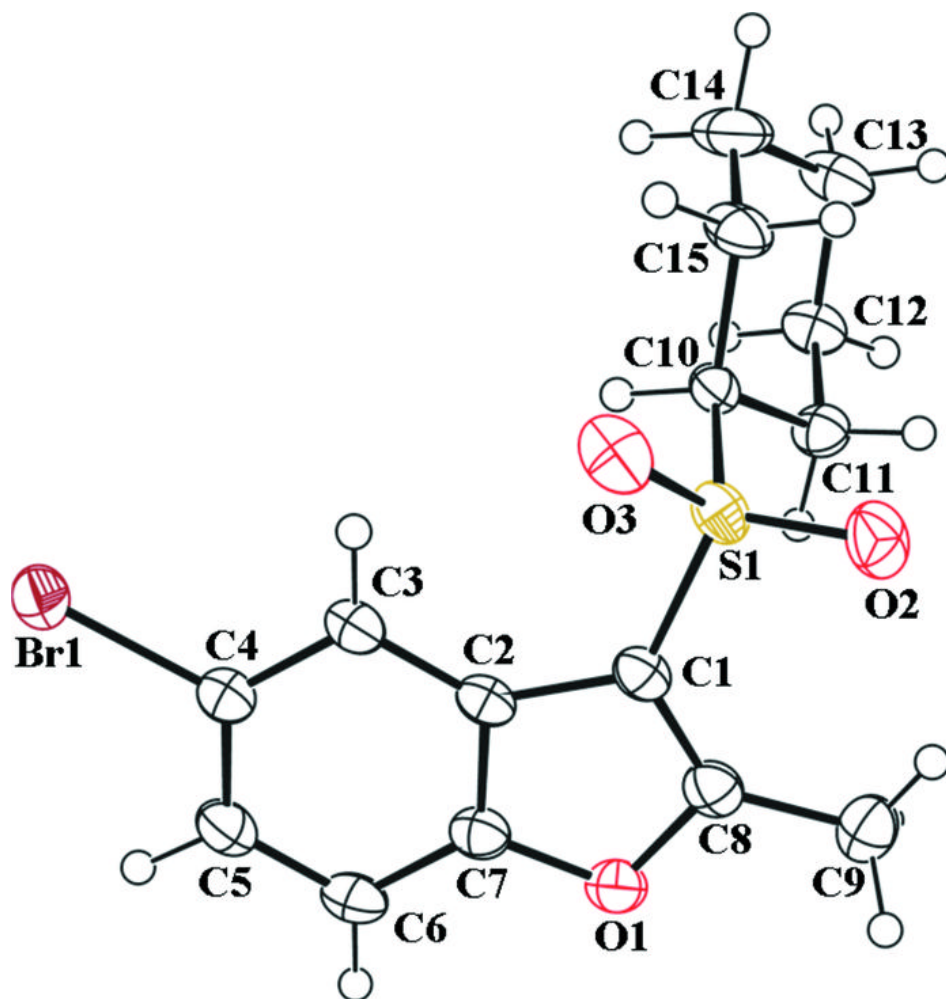


Fig. 2

