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5-Bromo-2-(4-fluorophenyl)-3-methylsulfinyl-1-benzofuran

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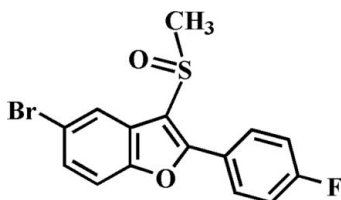
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.025; wR factor = 0.068; data-to-parameter ratio = 16.8.

In the title compound, $\text{C}_{15}\text{H}_{10}\text{BrFO}_2\text{S}$, the O atom and the methyl group of the methylsulfinyl substituent are located on opposite sides of the plane through the benzofuran fragment. The 4-fluorophenyl ring is rotated out of the benzofuran plane, as indicated by a dihedral angle of $26.23(5)^\circ$. The crystal structure is stabilized by a non-classical intermolecular C—H \cdots O hydrogen bond and a Br \cdots O halogen bond [3.163(2) Å].

Related literature

For the crystal structures of similar 2-(4-fluorophenyl)-3-methylsulfinyl-1-benzofuran derivatives, see: Choi *et al.* (2009*a,b*). For the pharmacological activity of benzofuran compounds, see: Howlett *et al.* (1999); Twyman & Allsop (1999). For natural products with benzofuran ring systems, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For a review of halogen bonding, see: Politzer *et al.* (2007).



Experimental

Crystal data

 $\text{C}_{15}\text{H}_{10}\text{BrFO}_2\text{S}$ $M_r = 353.20$

Triclinic, $P\bar{1}$
 $a = 7.8908(3)$ Å
 $b = 8.3434(3)$ Å
 $c = 10.8349(5)$ Å
 $\alpha = 94.886(2)^\circ$
 $\beta = 91.995(2)^\circ$
 $\gamma = 111.760(2)^\circ$

$V = 658.39(5)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 3.29$ mm⁻¹
 $T = 173$ K
 $0.27 \times 0.25 \times 0.24$ mm

Data collection

Bruker SMART APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.470$, $T_{\max} = 0.506$

11517 measured reflections
 3049 independent reflections
 2844 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.068$
 $S = 1.06$
 3049 reflections

182 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.46$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.41$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|-------|-------------|-------------|---------------|
| C14—H14 \cdots O2 ⁱ | 0.93 | 2.58 | 3.433 (3) | 153 |

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

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: OM2304).

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supporting information

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5-Bromo-2-(4-fluorophenyl)-3-methylsulfinyl-1-benzofuran

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

S1. Comment

Molecules including benzofuran moiety are of considerable interest due to a variety of their pharmacological activities (Howlett *et al.*, 1999; Twyman & Allsop, 1999) and these compounds are occurring in natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our continuing studies of the effect of side chain substituents on the solid state structures of 2-(4-fluorophenyl)-3-methylsulfinyl-1-benzofuran analogues (Choi *et al.*, 2009*a, b*), we report the crystal structure of the title compound (Fig. 1).

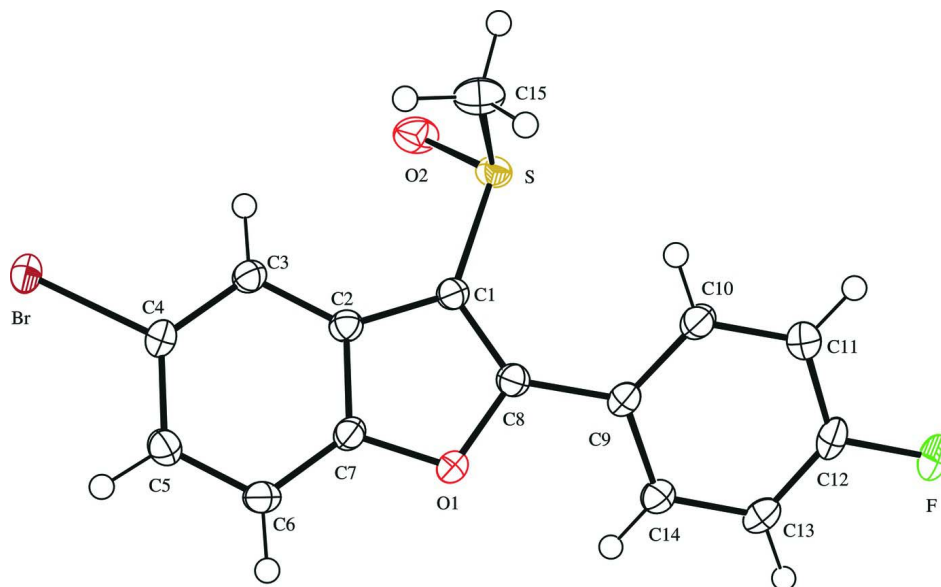
The benzofuran unit is essentially planar, with a mean deviation of 0.010 (2) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle formed by the plane of the benzofuran and the 4-fluorophenyl ring is 26.23 (5)°. The crystal packing (Fig. 2) is stabilized by a non-classical intermolecular C—H...O hydrogen bond between the 4-fluorophenyl H atom and the oxygen of the S=O unit, with a C14—H14...O2ⁱ (Table 1), and a Br...O halogen bond between the bromine and the oxygen of the S=O unit [Br...O2ⁱⁱ = 3.163 (2) Å; C—Br...O2ⁱⁱ = 173.37 (7)°] (Politzer *et al.*, 2007).

S2. Experimental

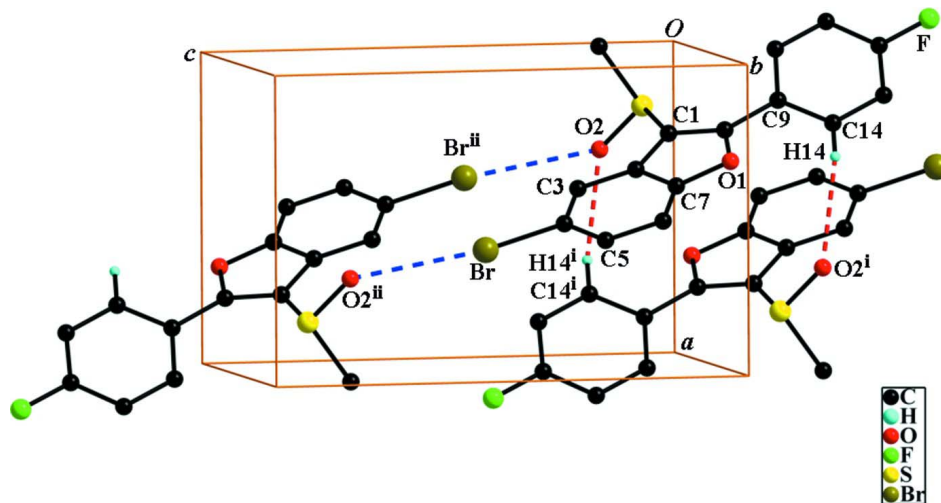
77% 3-Chloroperoxybenzoic acid (179 mg, 0.8 mmol) was added in small portions to a stirred solution of 5-bromo-2-(4-fluorophenyl)-3-methylsulfonyl-1-benzofuran (270 mg, 0.8 mmol) in dichloromethane (20 mL) at 273 K. After being stirred at room temperature for 3h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (hexane–ethyl acetate, 1:1 v/v) to afford the title compound as a colorless solid [yield 87%, m.p. 498–499 K; R_f = 0.6 (hexane-ethyl acetate, 1:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in chloroform at room temperature.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for aromatic H atoms and 0.96 Å for methyl H atoms, and with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H atoms and $1.5U_{eq}(C)$ 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

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

5-Bromo-2-(4-fluorophenyl)-3-methylsulfinyl-1-benzofuran

Crystal data

$C_{15}H_{10}BrFO_2S$

$M_r = 353.20$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 7.8908$ (3) Å

$b = 8.3434$ (3) Å

$c = 10.8349$ (5) Å

$\alpha = 94.886$ (2)°

$\beta = 91.995$ (2)°

$\gamma = 111.760$ (2)°

$V = 658.39$ (5) Å³

$Z = 2$

$F(000) = 352$

$D_x = 1.782$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 8308 reflections
 $\theta = 2.6\text{--}27.6^\circ$
 $\mu = 3.29 \text{ mm}^{-1}$

$T = 173 \text{ K}$
 Block, colourless
 $0.27 \times 0.25 \times 0.24 \text{ mm}$

Data collection

Bruker SMART APEXII CCD
 diffractometer
 Radiation source: Rotating Anode
 HELIOS monochromator
 Detector resolution: $10.0 \text{ pixels mm}^{-1}$
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.470$, $T_{\max} = 0.506$

11517 measured reflections
 3049 independent reflections
 2844 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\max} = 27.6^\circ$, $\theta_{\min} = 1.9^\circ$
 $h = -10 \rightarrow 10$
 $k = -10 \rightarrow 10$
 $l = -14 \rightarrow 13$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.068$
 $S = 1.06$
 3049 reflections
 182 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.3987P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.46 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.41 \text{ e \AA}^{-3}$

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> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|---------------|--------------|---------------|----------------------------------|
| Br | 0.59276 (3) | 0.78959 (2) | 0.522986 (16) | 0.02546 (8) |
| S | 0.18837 (6) | 0.20974 (6) | 0.09974 (4) | 0.02096 (11) |
| F | -0.07131 (19) | 0.23126 (17) | -0.50519 (11) | 0.0366 (3) |
| O1 | 0.33521 (19) | 0.67998 (17) | -0.01307 (12) | 0.0208 (3) |
| O2 | 0.3267 (2) | 0.18958 (19) | 0.18682 (15) | 0.0317 (3) |
| C1 | 0.2611 (3) | 0.4325 (2) | 0.07889 (17) | 0.0188 (3) |
| C2 | 0.3627 (2) | 0.5753 (2) | 0.17069 (17) | 0.0187 (3) |
| C3 | 0.4185 (3) | 0.5927 (2) | 0.29638 (17) | 0.0203 (4) |
| H3 | 0.3911 | 0.4969 | 0.3410 | 0.024* |
| C4 | 0.5166 (3) | 0.7593 (2) | 0.35152 (17) | 0.0206 (4) |
| C5 | 0.5612 (3) | 0.9066 (2) | 0.28757 (18) | 0.0224 (4) |
| H5 | 0.6287 | 1.0157 | 0.3287 | 0.027* |

| | | | | |
|------|-------------|------------|---------------|------------|
| C6 | 0.5049 (3) | 0.8900 (2) | 0.16288 (18) | 0.0222 (4) |
| H6 | 0.5320 | 0.9858 | 0.1183 | 0.027* |
| C7 | 0.4070 (3) | 0.7241 (2) | 0.10865 (16) | 0.0193 (3) |
| C8 | 0.2486 (2) | 0.5018 (2) | -0.02943 (17) | 0.0194 (3) |
| C9 | 0.1628 (3) | 0.4294 (2) | -0.15344 (16) | 0.0191 (3) |
| C10 | 0.0112 (3) | 0.2737 (3) | -0.17292 (18) | 0.0232 (4) |
| H10 | -0.0375 | 0.2150 | -0.1053 | 0.028* |
| C11 | -0.0679 (3) | 0.2050 (3) | -0.29139 (19) | 0.0251 (4) |
| H11 | -0.1676 | 0.1002 | -0.3045 | 0.030* |
| C12 | 0.0057 (3) | 0.2968 (3) | -0.38902 (17) | 0.0250 (4) |
| C13 | 0.1530 (3) | 0.4522 (3) | -0.37401 (18) | 0.0246 (4) |
| H13 | 0.1981 | 0.5111 | -0.4422 | 0.029* |
| C14 | 0.2329 (3) | 0.5193 (2) | -0.25552 (17) | 0.0213 (4) |
| H14 | 0.3329 | 0.6240 | -0.2436 | 0.026* |
| C15 | -0.0043 (3) | 0.1923 (3) | 0.1874 (2) | 0.0305 (4) |
| H15A | -0.0611 | 0.0755 | 0.2082 | 0.046* |
| H15B | -0.0908 | 0.2214 | 0.1389 | 0.046* |
| H15C | 0.0355 | 0.2705 | 0.2622 | 0.046* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Br | 0.03353 (13) | 0.02421 (11) | 0.01639 (11) | 0.00930 (8) | -0.00282 (7) | -0.00101 (7) |
| S | 0.0236 (2) | 0.0167 (2) | 0.0229 (2) | 0.00744 (17) | 0.00343 (17) | 0.00380 (17) |
| F | 0.0438 (8) | 0.0409 (7) | 0.0172 (6) | 0.0084 (6) | -0.0084 (5) | 0.0006 (5) |
| O1 | 0.0264 (7) | 0.0196 (6) | 0.0153 (6) | 0.0072 (5) | -0.0008 (5) | 0.0030 (5) |
| O2 | 0.0285 (8) | 0.0287 (7) | 0.0405 (9) | 0.0118 (6) | -0.0019 (6) | 0.0135 (6) |
| C1 | 0.0219 (9) | 0.0174 (8) | 0.0172 (8) | 0.0073 (7) | 0.0020 (7) | 0.0022 (6) |
| C2 | 0.0209 (9) | 0.0181 (8) | 0.0184 (8) | 0.0085 (7) | 0.0022 (7) | 0.0029 (7) |
| C3 | 0.0251 (9) | 0.0194 (8) | 0.0178 (8) | 0.0095 (7) | 0.0016 (7) | 0.0033 (7) |
| C4 | 0.0226 (9) | 0.0238 (9) | 0.0154 (8) | 0.0095 (7) | 0.0000 (7) | 0.0000 (7) |
| C5 | 0.0244 (9) | 0.0186 (8) | 0.0221 (9) | 0.0063 (7) | 0.0013 (7) | -0.0008 (7) |
| C6 | 0.0258 (9) | 0.0188 (8) | 0.0220 (9) | 0.0073 (7) | 0.0036 (7) | 0.0054 (7) |
| C7 | 0.0220 (9) | 0.0211 (8) | 0.0152 (8) | 0.0085 (7) | 0.0011 (7) | 0.0025 (7) |
| C8 | 0.0198 (9) | 0.0186 (8) | 0.0194 (8) | 0.0067 (7) | 0.0020 (7) | 0.0021 (7) |
| C9 | 0.0222 (9) | 0.0216 (9) | 0.0158 (8) | 0.0109 (7) | 0.0014 (7) | 0.0025 (7) |
| C10 | 0.0233 (9) | 0.0272 (9) | 0.0186 (9) | 0.0081 (8) | 0.0009 (7) | 0.0056 (7) |
| C11 | 0.0235 (9) | 0.0250 (9) | 0.0233 (9) | 0.0055 (8) | -0.0019 (7) | 0.0024 (7) |
| C12 | 0.0289 (10) | 0.0313 (10) | 0.0158 (9) | 0.0137 (8) | -0.0046 (7) | -0.0011 (7) |
| C13 | 0.0298 (10) | 0.0294 (10) | 0.0168 (9) | 0.0126 (8) | 0.0034 (7) | 0.0066 (7) |
| C14 | 0.0230 (9) | 0.0227 (9) | 0.0185 (9) | 0.0084 (7) | 0.0024 (7) | 0.0033 (7) |
| C15 | 0.0285 (10) | 0.0310 (10) | 0.0355 (11) | 0.0124 (9) | 0.0119 (9) | 0.0124 (9) |

Geometric parameters (Å, °)

| | | | |
|--------------------|-----------|-------|-----------|
| Br—C4 | 1.899 (2) | C6—C7 | 1.376 (3) |
| Br—O2 ⁱ | 3.163 (2) | C6—H6 | 0.9300 |
| S—O2 | 1.484 (2) | C8—C9 | 1.457 (3) |

| | | | |
|-----------------------|--------------|---------------|--------------|
| S—C1 | 1.767 (2) | C9—C10 | 1.395 (3) |
| S—C15 | 1.788 (2) | C9—C14 | 1.403 (3) |
| F—C12 | 1.355 (2) | C10—C11 | 1.385 (3) |
| O1—C8 | 1.379 (2) | C10—H10 | 0.9300 |
| O1—C7 | 1.381 (2) | C11—C12 | 1.376 (3) |
| C1—C8 | 1.368 (2) | C11—H11 | 0.9300 |
| C1—C2 | 1.445 (2) | C12—C13 | 1.375 (3) |
| C2—C3 | 1.395 (2) | C13—C14 | 1.385 (3) |
| C2—C7 | 1.397 (2) | C13—H13 | 0.9300 |
| C3—C4 | 1.385 (3) | C14—H14 | 0.9300 |
| C3—H3 | 0.9300 | C15—H15A | 0.9600 |
| C4—C5 | 1.399 (3) | C15—H15B | 0.9600 |
| C5—C6 | 1.386 (3) | C15—H15C | 0.9600 |
| C5—H5 | 0.9300 | | |
| | | | |
| C4—Br—O2 ⁱ | 173.37 (7) | C1—C8—C9 | 134.25 (17) |
| O2—S—C1 | 107.27 (9) | O1—C8—C9 | 115.24 (15) |
| O2—S—C15 | 106.10 (10) | C10—C9—C14 | 119.18 (17) |
| C1—S—C15 | 98.44 (9) | C10—C9—C8 | 121.53 (17) |
| C8—O1—C7 | 106.96 (14) | C14—C9—C8 | 119.28 (17) |
| C8—C1—C2 | 107.05 (16) | C11—C10—C9 | 121.04 (18) |
| C8—C1—S | 126.79 (14) | C11—C10—H10 | 119.5 |
| C2—C1—S | 125.87 (14) | C9—C10—H10 | 119.5 |
| C3—C2—C7 | 118.99 (17) | C12—C11—C10 | 117.90 (19) |
| C3—C2—C1 | 135.57 (17) | C12—C11—H11 | 121.0 |
| C7—C2—C1 | 105.44 (15) | C10—C11—H11 | 121.0 |
| C4—C3—C2 | 116.87 (16) | F—C12—C13 | 118.59 (18) |
| C4—C3—H3 | 121.6 | F—C12—C11 | 118.35 (18) |
| C2—C3—H3 | 121.6 | C13—C12—C11 | 123.06 (18) |
| C3—C4—C5 | 123.33 (17) | C12—C13—C14 | 118.82 (18) |
| C3—C4—Br | 118.36 (14) | C12—C13—H13 | 120.6 |
| C5—C4—Br | 118.31 (14) | C14—C13—H13 | 120.6 |
| C6—C5—C4 | 119.97 (17) | C13—C14—C9 | 119.98 (18) |
| C6—C5—H5 | 120.0 | C13—C14—H14 | 120.0 |
| C4—C5—H5 | 120.0 | C9—C14—H14 | 120.0 |
| C7—C6—C5 | 116.46 (17) | S—C15—H15A | 109.5 |
| C7—C6—H6 | 121.8 | S—C15—H15B | 109.5 |
| C5—C6—H6 | 121.8 | H15A—C15—H15B | 109.5 |
| C6—C7—O1 | 125.57 (16) | S—C15—H15C | 109.5 |
| C6—C7—C2 | 124.38 (17) | H15A—C15—H15C | 109.5 |
| O1—C7—C2 | 110.04 (15) | H15B—C15—H15C | 109.5 |
| C1—C8—O1 | 110.50 (16) | | |
| | | | |
| O2—S—C1—C8 | 141.05 (17) | C1—C2—C7—O1 | 1.3 (2) |
| C15—S—C1—C8 | -109.09 (18) | C2—C1—C8—O1 | -0.1 (2) |
| O2—S—C1—C2 | -31.88 (19) | S—C1—C8—O1 | -174.17 (13) |
| C15—S—C1—C2 | 77.98 (18) | C2—C1—C8—C9 | -178.79 (19) |
| C8—C1—C2—C3 | 178.7 (2) | S—C1—C8—C9 | 7.2 (3) |

| | | | |
|-------------|--------------|-----------------|--------------|
| S—C1—C2—C3 | -7.2 (3) | C7—O1—C8—C1 | 0.9 (2) |
| C8—C1—C2—C7 | -0.7 (2) | C7—O1—C8—C9 | 179.87 (15) |
| S—C1—C2—C7 | 173.40 (14) | C1—C8—C9—C10 | 26.6 (3) |
| C7—C2—C3—C4 | -0.4 (3) | O1—C8—C9—C10 | -152.03 (17) |
| C1—C2—C3—C4 | -179.7 (2) | C1—C8—C9—C14 | -154.2 (2) |
| C2—C3—C4—C5 | -0.3 (3) | O1—C8—C9—C14 | 27.2 (2) |
| C2—C3—C4—Br | 179.24 (13) | C14—C9—C10—C11 | 1.5 (3) |
| C3—C4—C5—C6 | 0.8 (3) | C8—C9—C10—C11 | -179.23 (18) |
| Br—C4—C5—C6 | -178.77 (14) | C9—C10—C11—C12 | -1.1 (3) |
| C4—C5—C6—C7 | -0.5 (3) | C10—C11—C12—F | -179.63 (17) |
| C5—C6—C7—O1 | 178.50 (17) | C10—C11—C12—C13 | 0.0 (3) |
| C5—C6—C7—C2 | -0.2 (3) | F—C12—C13—C14 | -179.66 (17) |
| C8—O1—C7—C6 | 179.73 (18) | C11—C12—C13—C14 | 0.7 (3) |
| C8—O1—C7—C2 | -1.4 (2) | C12—C13—C14—C9 | -0.3 (3) |
| C3—C2—C7—C6 | 0.7 (3) | C10—C9—C14—C13 | -0.8 (3) |
| C1—C2—C7—C6 | -179.82 (18) | C8—C9—C14—C13 | 179.95 (16) |
| C3—C2—C7—O1 | -178.21 (16) | | |

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

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C14—H14 \cdots O2 ⁱⁱ | 0.93 | 2.58 | 3.433 (3) | 153 |

Symmetry code: (ii) $-x+1, -y+1, -z$.