

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Propyl 2-(5-iodo-3-methylsulfinyl-1-benzofuran-2-yl)acetate

Hong Dae Choi,^a Pil Ja Seo,^a Byeng Wha Son^b and Uk Lee^{b*}^aDepartment of Chemistry, Donggeui University, San 24 Kaya-dong Busanjin-gu, Busan 614-714, Republic of Korea, and ^bDepartment 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

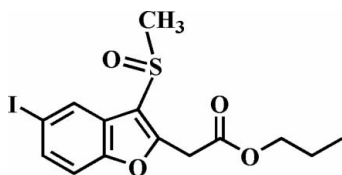
Received 8 December 2008; accepted 12 December 2008

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.029; wR factor = 0.069; data-to-parameter ratio = 16.3.

In the title compound, $\text{C}_{14}\text{H}_{15}\text{IO}_4\text{S}$, the O atom and the methyl group of the methylsulfinyl substituent lie on opposite sides of the plane of the benzofuran ring system. The crystal structure is stabilized by intermolecular $\text{C}-\text{H}\cdots\pi$ interactions between an H atom of the propyl methylene group closest to the carboxylate O atom and the benzene ring of a neighbouring molecule, and between an H atom of the outer propyl methylene group and the furan ring of a neighbouring molecule, respectively. Additionally, the crystal structure exhibits intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For the synthesis and crystal structures of similar alkyl 2-(5-iodo-3-methylsulfinyl-1-benzofuran-2-yl)acetate derivatives, see: Choi *et al.* (2007, 2008).



Experimental

Crystal data

 $\text{C}_{14}\text{H}_{15}\text{IO}_4\text{S}$ $M_r = 406.22$

Triclinic, $P\bar{1}$
 $a = 8.5468$ (4) Å
 $b = 10.0329$ (5) Å
 $c = 10.3239$ (5) Å
 $\alpha = 72.442$ (1)°
 $\beta = 81.345$ (1)°
 $\gamma = 65.088$ (1)°

$V = 765.21$ (6) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.24$ mm⁻¹
 $T = 293$ (2) K
 $0.30 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1999)
 $T_{\min} = 0.583$, $T_{\max} = 0.787$

6182 measured reflections
 2978 independent reflections
 2778 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.069$
 $S = 1.18$
 2982 reflections

183 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.52$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.56$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{C11}-\text{H11B}\cdots\text{Cg1}^{\text{i}}$ | 0.97 | 3.12 | 3.814 (4) | 130 |
| $\text{C12}-\text{H12B}\cdots\text{Cg2}^{\text{ii}}$ | 0.97 | 2.99 | 3.929 (3) | 162 |
| $\text{C3}-\text{H3}\cdots\text{O4}^{\text{iii}}$ | 0.93 | 2.60 | 3.468 (4) | 157 |
| $\text{C9}-\text{H9B}\cdots\text{O4}^{\text{iv}}$ | 0.97 | 2.40 | 3.356 (4) | 167 |

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x, -y+1, -z+2$. Cg1 and Cg2 are the centroids of the C2–C7 benzene ring and the C1/C2/C7/O1/C8 furan ring, respectively.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); 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: SJ2566).

References

- Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
 Bruker (2001). *SAINTE* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2007). *Acta Cryst.* **E63**, o4081.
 Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2008). *Acta Cryst.* **E64**, o2384.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Sheldrick, G. M. (1999). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2009). E65, o151 [doi:10.1107/S1600536808042359]

Propyl 2-(5-iodo-3-methylsulfinyl-1-benzofuran-2-yl)acetate

H. D. Choi, P. J. Seo, B. W. Son and U. Lee

Comment

This work is related to our previous communications on the synthesis and structure of alkyl 2-(5-iodo-3-methylsulfinyl-1-benzofuran-2-yl)acetate analogues, *viz.* ethyl 2-(5-iodo-3-methylsulfinyl-1-benzofuran-2-yl)acetate (Choi *et al.*, 2007) and isopropyl 2-(5-iodo-3-methylsulfinyl-1-benzofuran-2-yl)acetate (Choi *et al.*, 2008). Here we report the crystal structure of the title compound, propyl 2-(5-iodo-3-methylsulfinyl-1-benzofuran-2-yl)acetate (Fig. 1).

The benzofuran unit is essentially planar, with a mean deviation of 0.012 (2) Å from the least-squares plane defined by the nine constituent atoms. The molecular packing (Fig. 2) is stabilized by intermolecular C—H \cdots π interactions within each stack of molecules; one between the hydrogen of 11-methylene group and the benzene ring of the benzofuran unit, with a C11—H11B \cdots Cg1ⁱ separation of 3.12 Å, and a second between the hydrogen of 12-methylene group and the furan ring of the benzofuran unit, with a C12—H12B \cdots Cg2ⁱ with a separation of 2.99 Å (Table 1 and Fig. 2; Cg1 and Cg2 are the centroids of the C2–C7 benzene ring and the C1/C2/C7/O1/C8 furan ring, respectively, symmetry code as in Fig. 2). In addition, intermolecular C—H \cdots O hydrogen bonds in the structure are observed (Table 1).

Experimental

77% 3-chloroperoxybenzoic acid (173 mg, 0.77 mmol) was added in small portions to a stirred solution of propyl 2-(5-iodo-3-methylsulfonyl-1-benzofuran-2-yl)acetate (273 mg, 0.7 mmol) in dichloromethane (30 ml) at 273 K. After stirring for 3 h at room temperature, 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, 1:2 v/v) to afford the title compound as a colorless solid [yield 80%, m.p. 412–413 K; R_f = 0.58 (hexane-ethyl acetate, 1;2 v/v)]. Single crystals suitable for X-ray diffraction were prepared by evaporation of a solution of the title compound in acetone at room temperature. Spectroscopic analysis: ¹H NMR (CDCl₃, 400 MHz) δ 0.93 (t, J = 7.36 Hz, 3H), 1.64–1.72 (m, 2H), 3.07 (s, 3H), 4.02 (s, 2H), 4.11 (t, J = 6.60 Hz, 2H), 7.29 (d, J = 8.76 Hz, 1H), 7.66 (dd, J = 8.80 Hz and J = 1.84 Hz, 1H), 8.28 (d, J = 1.48 Hz, 1H); EI-MS 406 [M⁺].

Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for the aryl, 0.97 Å for the methylene, and 0.96 Å for the methyl H atoms. $U_{iso}(H)$ = 1.2 $U_{eq}(C)$ for the aryl and methylene H atoms, and 1.5 $U_{eq}(C)$ for methyl H atoms.

Figures

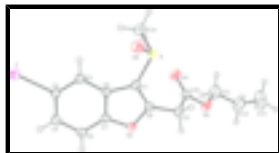


Fig. 1. The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level.

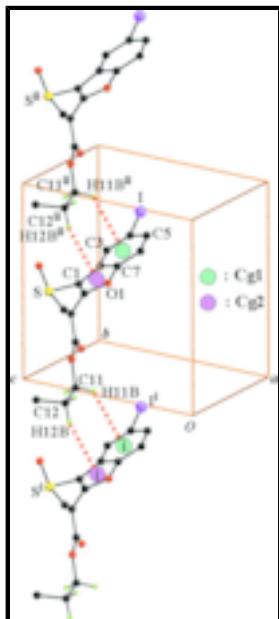


Fig. 2. C—H... π interactions (dotted lines) in the title compound. Cg denotes the ring centroid. [Symmetry code: (i) $x, y-1, z$; (ii) $x, y+1, z$.]

Propyl 2-(5-iodo-3-methylsulfinyl-1-benzofuran-2-yl)acetate

Crystal data

$C_{14}H_{15}IO_4S$

$M_r = 406.22$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.5468\ (4)\ \text{\AA}$

$b = 10.0329\ (5)\ \text{\AA}$

$c = 10.3239\ (5)\ \text{\AA}$

$\alpha = 72.442\ (1)^\circ$

$\beta = 81.345\ (1)^\circ$

$\gamma = 65.088\ (1)^\circ$

$V = 765.21\ (6)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 400$

$D_x = 1.763\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 4625 reflections

$\theta = 2.3\text{--}28.3^\circ$

$\mu = 2.24\ \text{mm}^{-1}$

$T = 293\ (2)\ \text{K}$

Plate, colorless

$0.30 \times 0.20 \times 0.10\ \text{mm}$

Data collection

Bruker SMART CCD
diffractometer

2982 independent reflections

Radiation source: fine-focus sealed tube

2778 reflections with $I > 2\sigma(I)$

Monochromator: graphite $R_{\text{int}} = 0.016$
 Detector resolution: 10.0 pixels mm^{-1} $\theta_{\text{max}} = 26.0^\circ$
 $T = 293(2)$ K $\theta_{\text{min}} = 2.3^\circ$
 φ and ω scans $h = -10 \rightarrow 10$
 Absorption correction: multi-scan (SADABS; Sheldrick, 1999) $k = -12 \rightarrow 12$
 $T_{\text{min}} = 0.583$, $T_{\text{max}} = 0.787$ $l = -12 \rightarrow 12$
 6182 measured reflections

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier map
 Least-squares matrix: full Hydrogen site location: difference Fourier map
 $R[F^2 > 2\sigma(F^2)] = 0.029$ H-atom parameters constrained
 $wR(F^2) = 0.069$ $w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 0.5734P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.18$ $(\Delta/\sigma)_{\text{max}} = 0.001$
 2982 reflections $\Delta\rho_{\text{max}} = 0.52 \text{ e } \text{Å}^{-3}$
 183 parameters $\Delta\rho_{\text{min}} = -0.56 \text{ e } \text{Å}^{-3}$
 Primary atom site location: structure-invariant direct methods Extinction correction: none

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 (Å^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|--------------|--------------|-------------|----------------------------------|
| I | 0.69366 (3) | 0.79269 (3) | 0.61486 (2) | 0.04832 (10) |
| S | 0.26183 (10) | 0.40380 (10) | 0.96397 (8) | 0.03932 (18) |
| O1 | 0.1660 (3) | 0.5368 (2) | 0.5730 (2) | 0.0350 (4) |
| O2 | 0.0455 (3) | 0.1416 (3) | 0.7355 (3) | 0.0530 (6) |
| O3 | 0.2911 (3) | 0.1379 (3) | 0.7896 (3) | 0.0567 (7) |
| O4 | 0.2582 (3) | 0.5257 (3) | 1.0206 (2) | 0.0529 (6) |
| C1 | 0.2539 (4) | 0.4770 (3) | 0.7857 (3) | 0.0337 (6) |
| C2 | 0.3414 (4) | 0.5677 (3) | 0.6976 (3) | 0.0303 (6) |
| C3 | 0.4622 (4) | 0.6215 (3) | 0.7127 (3) | 0.0335 (6) |
| H3 | 0.5072 | 0.5992 | 0.7969 | 0.040* |

supplementary materials

| | | | | |
|------|-------------|-------------|------------|-------------|
| C4 | 0.5121 (4) | 0.7091 (3) | 0.5973 (3) | 0.0340 (6) |
| C5 | 0.4466 (4) | 0.7459 (3) | 0.4690 (3) | 0.0387 (7) |
| H5 | 0.4825 | 0.8069 | 0.3943 | 0.046* |
| C6 | 0.3287 (4) | 0.6913 (3) | 0.4533 (3) | 0.0368 (7) |
| H6 | 0.2844 | 0.7134 | 0.3689 | 0.044* |
| C7 | 0.2796 (4) | 0.6029 (3) | 0.5682 (3) | 0.0322 (6) |
| C8 | 0.1529 (4) | 0.4619 (3) | 0.7075 (3) | 0.0330 (6) |
| C9 | 0.0405 (4) | 0.3755 (3) | 0.7359 (3) | 0.0367 (7) |
| H9A | -0.0360 | 0.4135 | 0.6606 | 0.044* |
| H9B | -0.0303 | 0.3929 | 0.8168 | 0.044* |
| C10 | 0.1438 (4) | 0.2060 (4) | 0.7564 (3) | 0.0396 (7) |
| C11 | 0.1272 (5) | -0.0221 (4) | 0.7496 (6) | 0.0702 (13) |
| H11A | 0.1879 | -0.0747 | 0.8343 | 0.084* |
| H11B | 0.2094 | -0.0435 | 0.6752 | 0.084* |
| C12 | -0.0126 (6) | -0.0740 (5) | 0.7479 (5) | 0.0683 (12) |
| H12A | -0.0746 | -0.0170 | 0.6641 | 0.082* |
| H12B | 0.0396 | -0.1808 | 0.7486 | 0.082* |
| C13 | -0.1370 (9) | -0.0548 (7) | 0.8641 (6) | 0.102 (2) |
| H13A | -0.0787 | -0.1189 | 0.9471 | 0.154* |
| H13B | -0.2278 | -0.0829 | 0.8536 | 0.154* |
| H13C | -0.1850 | 0.0497 | 0.8670 | 0.154* |
| C14 | 0.4798 (5) | 0.2651 (4) | 0.9739 (4) | 0.0539 (9) |
| H14A | 0.5572 | 0.3159 | 0.9444 | 0.081* |
| H14B | 0.4958 | 0.2005 | 0.9166 | 0.081* |
| H14C | 0.5031 | 0.2045 | 1.0661 | 0.081* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|---------------|---------------|
| I | 0.04655 (14) | 0.04768 (14) | 0.05934 (16) | -0.02881 (11) | -0.00540 (10) | -0.00948 (10) |
| S | 0.0427 (4) | 0.0487 (4) | 0.0301 (4) | -0.0235 (4) | -0.0015 (3) | -0.0075 (3) |
| O1 | 0.0358 (11) | 0.0404 (11) | 0.0329 (11) | -0.0184 (9) | -0.0071 (8) | -0.0077 (9) |
| O2 | 0.0399 (12) | 0.0362 (12) | 0.0874 (19) | -0.0165 (10) | -0.0083 (12) | -0.0177 (12) |
| O3 | 0.0393 (13) | 0.0466 (14) | 0.0806 (19) | -0.0156 (11) | -0.0146 (12) | -0.0079 (13) |
| O4 | 0.0619 (16) | 0.0638 (16) | 0.0409 (13) | -0.0264 (13) | -0.0003 (11) | -0.0234 (12) |
| C1 | 0.0349 (15) | 0.0350 (15) | 0.0336 (15) | -0.0152 (13) | -0.0026 (12) | -0.0098 (12) |
| C2 | 0.0314 (14) | 0.0304 (14) | 0.0297 (14) | -0.0112 (12) | -0.0026 (11) | -0.0099 (11) |
| C3 | 0.0360 (15) | 0.0335 (15) | 0.0339 (16) | -0.0142 (12) | -0.0052 (12) | -0.0104 (12) |
| C4 | 0.0316 (15) | 0.0311 (14) | 0.0419 (16) | -0.0131 (12) | -0.0016 (12) | -0.0119 (13) |
| C5 | 0.0400 (17) | 0.0335 (15) | 0.0377 (16) | -0.0138 (13) | 0.0009 (13) | -0.0049 (13) |
| C6 | 0.0392 (16) | 0.0395 (16) | 0.0301 (15) | -0.0150 (13) | -0.0048 (12) | -0.0062 (13) |
| C7 | 0.0299 (14) | 0.0311 (14) | 0.0378 (15) | -0.0111 (12) | -0.0053 (12) | -0.0118 (12) |
| C8 | 0.0339 (15) | 0.0320 (15) | 0.0335 (15) | -0.0142 (12) | -0.0027 (12) | -0.0070 (12) |
| C9 | 0.0343 (15) | 0.0412 (16) | 0.0410 (17) | -0.0188 (13) | -0.0023 (13) | -0.0134 (13) |
| C10 | 0.0397 (17) | 0.0422 (17) | 0.0403 (17) | -0.0220 (14) | 0.0007 (13) | -0.0082 (14) |
| C11 | 0.051 (2) | 0.038 (2) | 0.122 (4) | -0.0153 (17) | -0.001 (2) | -0.027 (2) |
| C12 | 0.063 (3) | 0.043 (2) | 0.105 (4) | -0.0231 (19) | -0.004 (2) | -0.026 (2) |
| C13 | 0.124 (5) | 0.100 (4) | 0.111 (5) | -0.078 (4) | 0.044 (4) | -0.040 (4) |

C14 0.051 (2) 0.055 (2) 0.049 (2) -0.0147 (17) -0.0128 (16) -0.0084 (17)

Geometric parameters (Å, °)

| | | | |
|------------|-------------|---------------|-----------|
| I—C4 | 2.102 (3) | C6—C7 | 1.379 (4) |
| S—O4 | 1.494 (3) | C6—H6 | 0.9300 |
| S—C1 | 1.764 (3) | C8—C9 | 1.491 (4) |
| S—C14 | 1.790 (4) | C9—C10 | 1.513 (4) |
| O1—C7 | 1.375 (3) | C9—H9A | 0.9700 |
| O1—C8 | 1.378 (3) | C9—H9B | 0.9700 |
| O2—C10 | 1.329 (4) | C11—C12 | 1.495 (6) |
| O2—C11 | 1.458 (4) | C11—H11A | 0.9700 |
| O3—C10 | 1.197 (4) | C11—H11B | 0.9700 |
| C1—C8 | 1.347 (4) | C12—C13 | 1.480 (7) |
| C1—C2 | 1.443 (4) | C12—H12A | 0.9700 |
| C2—C3 | 1.397 (4) | C12—H12B | 0.9700 |
| C2—C7 | 1.399 (4) | C13—H13A | 0.9600 |
| C3—C4 | 1.380 (4) | C13—H13B | 0.9600 |
| C3—H3 | 0.9300 | C13—H13C | 0.9600 |
| C4—C5 | 1.400 (4) | C14—H14A | 0.9600 |
| C5—C6 | 1.381 (4) | C14—H14B | 0.9600 |
| C5—H5 | 0.9300 | C14—H14C | 0.9600 |
| O4—S—C1 | 106.92 (14) | C10—C9—H9A | 109.1 |
| O4—S—C14 | 106.66 (17) | C8—C9—H9B | 109.1 |
| C1—S—C14 | 98.06 (16) | C10—C9—H9B | 109.1 |
| C7—O1—C8 | 106.0 (2) | H9A—C9—H9B | 107.9 |
| C10—O2—C11 | 116.8 (3) | O3—C10—O2 | 124.3 (3) |
| C8—C1—C2 | 107.3 (3) | O3—C10—C9 | 125.7 (3) |
| C8—C1—S | 123.9 (2) | O2—C10—C9 | 110.0 (3) |
| C2—C1—S | 128.7 (2) | O2—C11—C12 | 107.4 (3) |
| C3—C2—C7 | 119.1 (3) | O2—C11—H11A | 110.2 |
| C3—C2—C1 | 136.3 (3) | C12—C11—H11A | 110.2 |
| C7—C2—C1 | 104.6 (2) | O2—C11—H11B | 110.2 |
| C4—C3—C2 | 117.2 (3) | C12—C11—H11B | 110.2 |
| C4—C3—H3 | 121.4 | H11A—C11—H11B | 108.5 |
| C2—C3—H3 | 121.4 | C13—C12—C11 | 113.5 (4) |
| C3—C4—C5 | 123.1 (3) | C13—C12—H12A | 108.9 |
| C3—C4—I | 118.6 (2) | C11—C12—H12A | 108.9 |
| C5—C4—I | 118.3 (2) | C13—C12—H12B | 108.9 |
| C6—C5—C4 | 119.9 (3) | C11—C12—H12B | 108.9 |
| C6—C5—H5 | 120.1 | H12A—C12—H12B | 107.7 |
| C4—C5—H5 | 120.1 | C12—C13—H13A | 109.5 |
| C7—C6—C5 | 117.2 (3) | C12—C13—H13B | 109.5 |
| C7—C6—H6 | 121.4 | H13A—C13—H13B | 109.5 |
| C5—C6—H6 | 121.4 | C12—C13—H13C | 109.5 |
| O1—C7—C6 | 125.8 (3) | H13A—C13—H13C | 109.5 |
| O1—C7—C2 | 110.7 (3) | H13B—C13—H13C | 109.5 |
| C6—C7—C2 | 123.6 (3) | S—C14—H14A | 109.5 |
| C1—C8—O1 | 111.4 (3) | S—C14—H14B | 109.5 |

supplementary materials

| | | | |
|-------------|------------|----------------|------------|
| C1—C8—C9 | 133.3 (3) | H14A—C14—H14B | 109.5 |
| O1—C8—C9 | 115.2 (2) | S—C14—H14C | 109.5 |
| C8—C9—C10 | 112.3 (2) | H14A—C14—H14C | 109.5 |
| C8—C9—H9A | 109.1 | H14B—C14—H14C | 109.5 |
| O4—S—C1—C8 | -135.7 (3) | C3—C2—C7—O1 | 178.3 (2) |
| C14—S—C1—C8 | 114.1 (3) | C1—C2—C7—O1 | -1.5 (3) |
| O4—S—C1—C2 | 40.8 (3) | C3—C2—C7—C6 | -1.4 (4) |
| C14—S—C1—C2 | -69.4 (3) | C1—C2—C7—C6 | 178.8 (3) |
| C8—C1—C2—C3 | -178.7 (3) | C2—C1—C8—O1 | -0.3 (3) |
| S—C1—C2—C3 | 4.4 (5) | S—C1—C8—O1 | 176.8 (2) |
| C8—C1—C2—C7 | 1.0 (3) | C2—C1—C8—C9 | 175.8 (3) |
| S—C1—C2—C7 | -175.9 (2) | S—C1—C8—C9 | -7.1 (5) |
| C7—C2—C3—C4 | 0.8 (4) | C7—O1—C8—C1 | -0.6 (3) |
| C1—C2—C3—C4 | -179.4 (3) | C7—O1—C8—C9 | -177.5 (2) |
| C2—C3—C4—C5 | 0.4 (4) | C1—C8—C9—C10 | -74.2 (4) |
| C2—C3—C4—I | -180.0 (2) | O1—C8—C9—C10 | 101.8 (3) |
| C3—C4—C5—C6 | -1.2 (5) | C11—O2—C10—O3 | -2.4 (5) |
| I—C4—C5—C6 | 179.2 (2) | C11—O2—C10—C9 | 179.2 (3) |
| C4—C5—C6—C7 | 0.7 (4) | C8—C9—C10—O3 | 22.6 (5) |
| C8—O1—C7—C6 | -179.0 (3) | C8—C9—C10—O2 | -159.0 (3) |
| C8—O1—C7—C2 | 1.3 (3) | C10—O2—C11—C12 | 169.5 (4) |
| C5—C6—C7—O1 | -179.1 (3) | O2—C11—C12—C13 | -63.9 (6) |
| C5—C6—C7—C2 | 0.6 (4) | | |

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------------------|-------|-------------|-------------|---------------|
| C11—H11B \cdots Cg1 ⁱ | 0.97 | 3.12 | 3.814 (4) | 130 |
| C12—H12B \cdots Cg2 ⁱⁱ | 0.97 | 2.99 | 3.929 (3) | 162 |
| C3—H3 \cdots O4 ⁱⁱⁱ | 0.93 | 2.60 | 3.468 (4) | 157 |
| C9—H9B \cdots O4 ^{iv} | 0.97 | 2.40 | 3.356 (4) | 167 |

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

Fig. 1

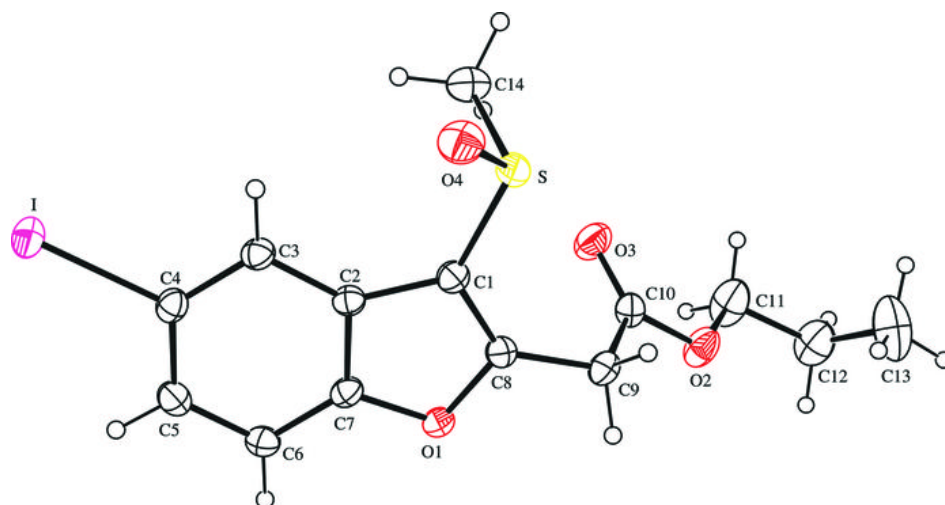


Fig. 2

