# organic compounds

# 3-(4-Bromophenylsulfonyl)-5-cyclopentyl-2-methyl-1-benzofuran

## Hong Dae Choi,a Pil Ja Seoa and Uk Leeb*

aDepartment of Chemistry, Dongeui 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

In the title compound, $C_{20}H_{19}BrO_3S$, the cyclopentyl ring adopts an envelope conformation. The 4-bromophenyl ring makes a dihedral angle of 82.09 (6)° with the mean plane [mean deviation = 0.026 (2) Å] of the benzofuran fragment. In the crystal, molecules are linked by weak C—H⋯O hydrogen bonds and Br⋯O contacts [3.309 (2) Å].

## Related literature

For background information and the crystal structure of a related compound, see: Seo *et al.* (2011). For a review of halogen bonding, see: Politzer *et al.* (2007).
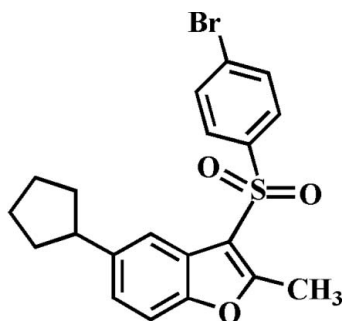


## Experimental

### Crystal data

| | |
|---|---|
| $C_{20}H_{19}BrO_3S$ | $V$ = 1844.69 (7) Å³ |
| $M_r$ = 419.32 | $Z$ = 4 |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a$ = 6.8956 (2) Å | $\mu$ = 2.36 mm⁻¹ |
| $b$ = 17.1034 (3) Å | $T$ = 173 K |
| $c$ = 15.7773 (3) Å | 0.38 × 0.34 × 0.27 mm |
| $\beta$ = 97.533 (1)° | |

### Data collection

| | |
|---|---|
| Bruker SMART APEXII CCD diffractometer | 18310 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | 4602 independent reflections |
| | 3416 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.469, $T_{max}$ = 0.570 | $R_{int}$ = 0.041 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.038 | 227 parameters |
| $wR(F^2)$ = 0.093 | H-atom parameters constrained |
| $S$ = 1.02 | $\Delta\rho_{max}$ = 0.58 e Å⁻³ |
| 4602 reflections | $\Delta\rho_{min}$ = −0.73 e Å⁻³ |

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C17—H17⋯O2i | 0.95 | 2.51 | 3.169 (3) | 126 |

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

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*.

## References

Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2009). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Politzer, P., Lane, P., Concha, M. C., Ma, Y. & Murray, J. S. (2007). *J. Mol. Model.* **13**, 305-311.
Seo, P. J., Choi, H. D., Son, B. W. & Lee, U. (2011). *Acta Cryst.* E**67**, o2223.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supplementary materials

## 3-(4-Bromophenylsulfonyl)-5-cyclopentyl-2-methyl-1-benzofuran

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

### Comment

As a part of our ongoing study of 5-cyclopentyl-2-methyl-1-benzofuran derivatives containing a 3-phenylsulfonyl substituent (Seo *et al.*, 2011), 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 0.026 (2) Å from the least-squares plane defined by the nine constituent atoms. The cyclopentyl ring has an envelope conformtion. The dihedral angle between the 4-bromophenyl ring and the mean plane of the benzofurn fragment is 82.09 (6)°. In the crystal structure (Fig. 2), molecules are connected by weak C—H···O interactions (Table 1). The crystal packing (Fig. 2) also exhibits Br···O halogen-bonding interactions between the bromine atom and the O atom of the O=S=O unit [Br1···O3$^i$ = 3.309 (2) Å, C18—Br1···O3$^i$ = 153.82 (8)°] (Politzer *et al.*, 2007).

### Experimental

3-Chloroperoxybenzoic acid (77%, 381 mg, 1.7 mmol) was added in small portions to a stirred solution of 3-(4-bromo-phenylsulfanyl)-5-cyclopentyl-2-methyl-1-benzofuran (310 mg, 0.8 mmol) in dichloromethane (30 mL) at 273 K. After being stirred at room temperature for 10 h, 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 71%, m.p. 423–424 K; $R_f$ = 0.48 (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.

### Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for the aryl, 1.00 Å for the methine, 0.99 Å for the methylene, and 0.98 Å for the methyl H atoms. $U_{iso}$(H) = 1.2$U_{eq}$(C) for the aryl, methine, and methylene H atoms, and 1.5$U_{eq}$(C) for the methyl H atoms. The positions of methyl hydrogens were optimized rotationally.

### Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); 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* (Sheldrick, 2008).
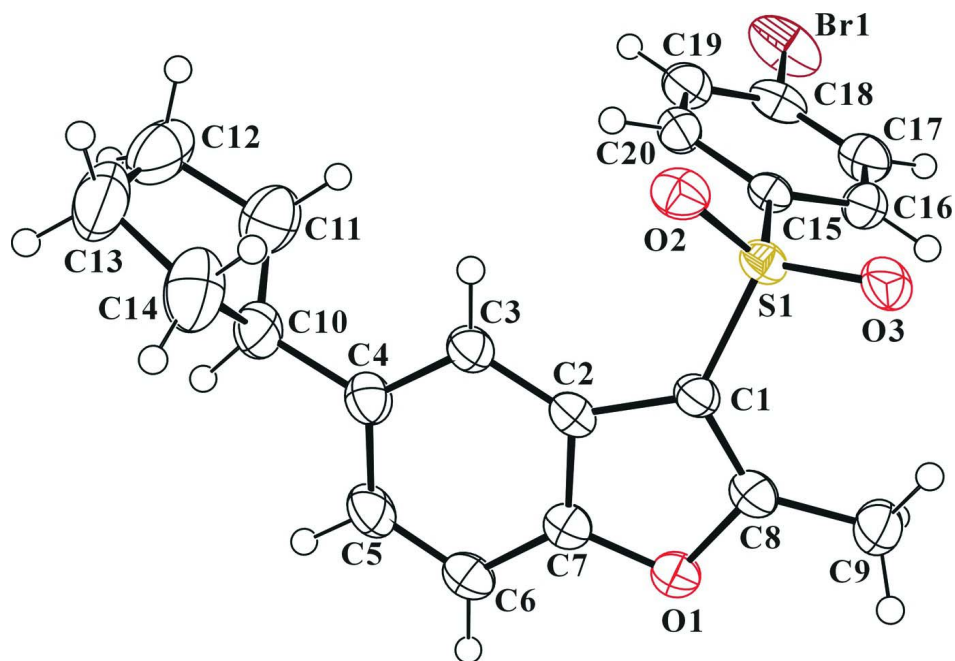
**Figure 1**

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.
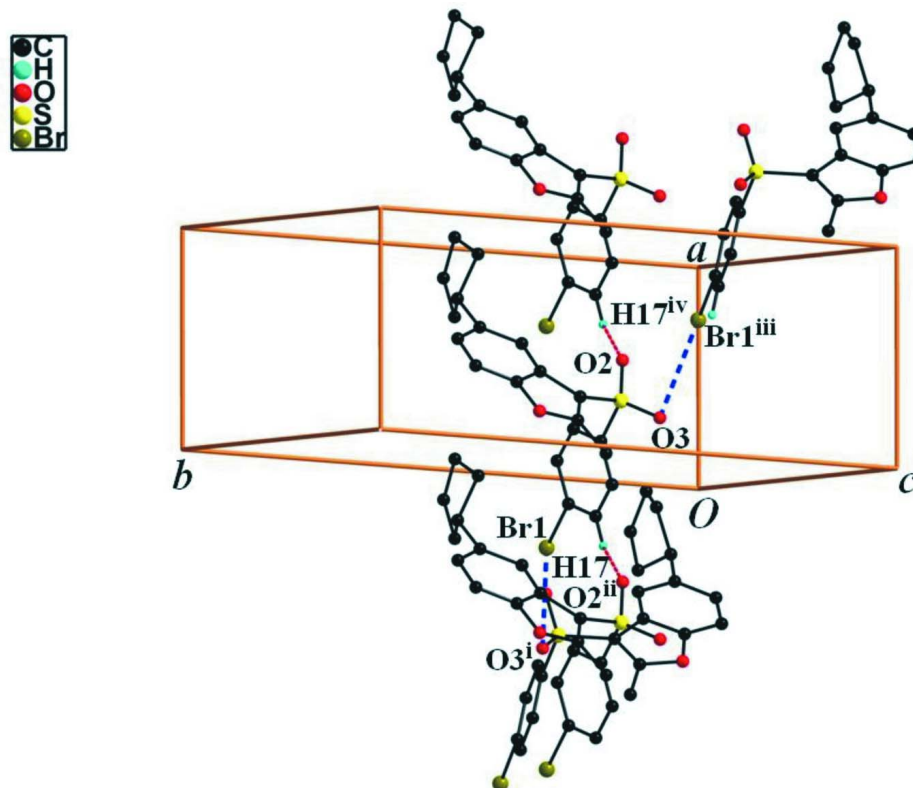
**Figure 2**

A view of the C—H···O and Br···O interactions (dotted lines) in the crystal structure of the title compound. H atoms not participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i) $x - 1$, $-y + 1/2$, $z - 1/2$; (ii) $x + 1$, $y$, $z$; (iii) $x + 1$, $-y + 1/2$, $z + 1/2$; (iv) $x + 1$, y, z.]

**3-(4-Bromophenylsulfonyl)-5-cyclopentyl-2-methyl-1-benzofuran**

*Crystal data*

| | |
|---|---|
| $C_{20}H_{19}BrO_3S$ | $F(000) = 856$ |
| $M_r = 419.32$ | $D_x = 1.510$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 5006 reflections |
| $a = 6.8956$ (2) Å | $\theta = 2.4–26.9°$ |
| $b = 17.1034$ (3) Å | $\mu = 2.36$ mm$^{-1}$ |
| $c = 15.7773$ (3) Å | $T = 173$ K |
| $\beta = 97.533$ (1)° | Block, colourless |
| $V = 1844.69$ (7) Å$^3$ | $0.38 \times 0.34 \times 0.27$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD diffractometer | Absorption correction: multi-scan (*SADABS*; Bruker, 2009) |
| Radiation source: rotating anode | $T_{min} = 0.469$, $T_{max} = 0.570$ |
| Graphite multilayer monochromator | 18310 measured reflections |
| Detector resolution: 10.0 pixels mm$^{-1}$ | 4602 independent reflections |
| $\varphi$ and $\omega$ scans | 3416 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.041$ |

$\theta_{max} = 28.4°$, $\theta_{min} = 1.8°$

$h = -9→9$

$k = -22→22$

$l = -21→19$

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | Hydrogen site location: difference Fourier map |
| $wR(F^2) = 0.093$ | H-atom parameters constrained |
| $S = 1.02$ | $w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.8231P]$ |
| 4602 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 227 parameters | $(\Delta/\sigma)_{max} < 0.001$ |
| 0 restraints | $\Delta\rho_{max} = 0.58$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{min} = -0.73$ 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | −0.32092 (5) | 0.301064 (16) | 0.016006 (19) | 0.06550 (13) |
| S1 | 0.31357 (7) | 0.28508 (3) | 0.34905 (3) | 0.02688 (12) |
| O1 | 0.2226 (2) | 0.48448 (8) | 0.45861 (10) | 0.0398 (4) |
| O2 | 0.5019 (2) | 0.27163 (8) | 0.32240 (10) | 0.0356 (3) |
| O3 | 0.2418 (2) | 0.23232 (8) | 0.40858 (9) | 0.0363 (3) |
| C1 | 0.3124 (3) | 0.37925 (11) | 0.38922 (12) | 0.0282 (4) |
| C2 | 0.4174 (3) | 0.44557 (11) | 0.36055 (13) | 0.0288 (4) |
| C3 | 0.5464 (3) | 0.45853 (11) | 0.30148 (13) | 0.0313 (4) |
| H3 | 0.5924 | 0.4161 | 0.2707 | 0.038* |
| C4 | 0.6077 (3) | 0.53476 (12) | 0.28803 (14) | 0.0351 (5) |
| C5 | 0.5410 (4) | 0.59592 (12) | 0.33602 (15) | 0.0406 (5) |
| H5 | 0.5841 | 0.6476 | 0.3268 | 0.049* |
| C6 | 0.4158 (4) | 0.58411 (12) | 0.39592 (15) | 0.0408 (5) |
| H6 | 0.3735 | 0.6259 | 0.4286 | 0.049* |
| C7 | 0.3554 (3) | 0.50843 (12) | 0.40580 (14) | 0.0338 (5) |
| C8 | 0.1965 (3) | 0.40590 (12) | 0.44621 (14) | 0.0351 (5) |
| C9 | 0.0490 (4) | 0.36946 (14) | 0.49391 (18) | 0.0509 (7) |
| H9A | −0.0824 | 0.3813 | 0.4652 | 0.076* |
| H9B | 0.0634 | 0.3903 | 0.5523 | 0.076* |
| H9C | 0.0685 | 0.3127 | 0.4959 | 0.076* |
| C10 | 0.7396 (4) | 0.55251 (12) | 0.22173 (16) | 0.0426 (6) |
| H10 | 0.7525 | 0.6106 | 0.2187 | 0.051* |
| C11 | 0.6704 (5) | 0.52353 (19) | 0.13200 (18) | 0.0642 (8) |
| H11A | 0.5648 | 0.5574 | 0.1037 | 0.077* |

| | | | |
|---|---|---|---|
| H11B | 0.6206 | 0.4693 | 0.1334 | 0.077* |
| C12 | 0.8493 (6) | 0.52695 (18) | 0.0848 (2) | 0.0763 (11) |
| H12A | 0.8563 | 0.4797 | 0.0491 | 0.092* |
| H12B | 0.8435 | 0.5736 | 0.0474 | 0.092* |
| C13 | 1.0259 (6) | 0.53131 (18) | 0.1533 (3) | 0.0822 (12) |
| H13A | 1.0902 | 0.5830 | 0.1525 | 0.099* |
| H13B | 1.1222 | 0.4902 | 0.1443 | 0.099* |
| C14 | 0.9451 (4) | 0.5187 (2) | 0.2377 (2) | 0.0685 (9) |
| H14A | 0.9416 | 0.4623 | 0.2519 | 0.082* |
| H14B | 1.0253 | 0.5465 | 0.2850 | 0.082* |
| C15 | 0.1402 (3) | 0.28833 (10) | 0.25667 (12) | 0.0257 (4) |
| C16 | −0.0527 (3) | 0.26893 (12) | 0.26253 (14) | 0.0339 (5) |
| H16 | −0.0905 | 0.2530 | 0.3157 | 0.041* |
| C17 | −0.1896 (3) | 0.27292 (13) | 0.19020 (15) | 0.0402 (5) |
| H17 | −0.3224 | 0.2596 | 0.1931 | 0.048* |
| C18 | −0.1312 (3) | 0.29636 (12) | 0.11402 (15) | 0.0377 (5) |
| C19 | 0.0603 (4) | 0.31567 (12) | 0.10699 (14) | 0.0382 (5) |
| H19 | 0.0971 | 0.3315 | 0.0536 | 0.046* |
| C20 | 0.1983 (3) | 0.31153 (11) | 0.17929 (13) | 0.0318 (4) |
| H20 | 0.3311 | 0.3244 | 0.1760 | 0.038* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0750 (2) | 0.04795 (17) | 0.0610 (2) | 0.00540 (13) | −0.03790 (16) | −0.00334 (12) |
| S1 | 0.0311 (3) | 0.0203 (2) | 0.0284 (2) | 0.00110 (17) | 0.00070 (19) | −0.00012 (18) |
| O1 | 0.0528 (10) | 0.0260 (7) | 0.0438 (9) | −0.0022 (6) | 0.0187 (8) | −0.0062 (6) |
| O2 | 0.0312 (8) | 0.0323 (7) | 0.0424 (9) | 0.0064 (6) | 0.0021 (7) | −0.0042 (6) |
| O3 | 0.0500 (10) | 0.0247 (7) | 0.0336 (8) | −0.0015 (6) | 0.0034 (7) | 0.0042 (6) |
| C1 | 0.0340 (11) | 0.0227 (9) | 0.0277 (10) | −0.0017 (8) | 0.0030 (8) | −0.0015 (8) |
| C2 | 0.0317 (11) | 0.0228 (9) | 0.0306 (10) | −0.0021 (7) | −0.0001 (8) | −0.0017 (7) |
| C3 | 0.0334 (12) | 0.0258 (10) | 0.0349 (11) | −0.0007 (8) | 0.0050 (9) | −0.0013 (8) |
| C4 | 0.0371 (13) | 0.0282 (10) | 0.0402 (12) | −0.0016 (8) | 0.0057 (9) | 0.0031 (9) |
| C5 | 0.0473 (14) | 0.0229 (10) | 0.0526 (14) | −0.0043 (9) | 0.0098 (11) | −0.0004 (9) |
| C6 | 0.0527 (15) | 0.0246 (10) | 0.0466 (13) | −0.0029 (9) | 0.0114 (11) | −0.0071 (9) |
| C7 | 0.0382 (13) | 0.0291 (10) | 0.0346 (11) | −0.0018 (8) | 0.0068 (9) | −0.0031 (8) |
| C8 | 0.0435 (13) | 0.0246 (10) | 0.0377 (12) | −0.0023 (8) | 0.0072 (9) | −0.0026 (8) |
| C9 | 0.0638 (18) | 0.0349 (12) | 0.0610 (16) | −0.0046 (11) | 0.0349 (14) | −0.0037 (11) |
| C10 | 0.0514 (15) | 0.0244 (10) | 0.0551 (15) | −0.0008 (9) | 0.0188 (12) | 0.0070 (10) |
| C11 | 0.076 (2) | 0.0694 (19) | 0.0507 (17) | −0.0048 (15) | 0.0195 (15) | 0.0125 (14) |
| C12 | 0.113 (3) | 0.0466 (16) | 0.082 (2) | 0.0057 (17) | 0.061 (2) | 0.0127 (15) |
| C13 | 0.075 (2) | 0.0528 (18) | 0.132 (3) | −0.0021 (16) | 0.065 (3) | 0.0032 (19) |
| C14 | 0.0474 (18) | 0.072 (2) | 0.088 (2) | −0.0004 (14) | 0.0185 (16) | 0.0145 (17) |
| C15 | 0.0281 (11) | 0.0196 (8) | 0.0291 (10) | 0.0022 (7) | 0.0027 (8) | −0.0020 (7) |
| C16 | 0.0303 (12) | 0.0347 (11) | 0.0378 (12) | −0.0025 (8) | 0.0083 (9) | −0.0032 (9) |
| C17 | 0.0283 (12) | 0.0408 (12) | 0.0502 (14) | −0.0009 (9) | 0.0006 (10) | −0.0085 (10) |
| C18 | 0.0420 (14) | 0.0276 (10) | 0.0389 (12) | 0.0057 (8) | −0.0117 (10) | −0.0069 (9) |
| C19 | 0.0542 (15) | 0.0315 (11) | 0.0279 (11) | −0.0023 (9) | 0.0014 (10) | 0.0011 (8) |
| C20 | 0.0332 (12) | 0.0295 (10) | 0.0329 (11) | −0.0035 (8) | 0.0041 (9) | −0.0007 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C18 | 1.892 (2) | C10—C11 | 1.517 (4) |
| Br1—O3ⁱ | 3.3090 (16) | C10—C14 | 1.521 (4) |
| S1—O2 | 1.4348 (15) | C10—H10 | 1.0000 |
| S1—O3 | 1.4362 (15) | C11—C12 | 1.523 (4) |
| S1—C1 | 1.7313 (19) | C11—H11A | 0.9900 |
| S1—C15 | 1.760 (2) | C11—H11B | 0.9900 |
| O1—C8 | 1.367 (2) | C12—C13 | 1.520 (5) |
| O1—C7 | 1.379 (3) | C12—H12A | 0.9900 |
| C1—C8 | 1.358 (3) | C12—H12B | 0.9900 |
| C1—C2 | 1.449 (3) | C13—C14 | 1.525 (4) |
| C2—C3 | 1.388 (3) | C13—H13A | 0.9900 |
| C2—C7 | 1.388 (3) | C13—H13B | 0.9900 |
| C3—C4 | 1.395 (3) | C14—H14A | 0.9900 |
| C3—H3 | 0.9500 | C14—H14B | 0.9900 |
| C4—C5 | 1.404 (3) | C15—C16 | 1.386 (3) |
| C4—C10 | 1.504 (3) | C15—C20 | 1.392 (3) |
| C5—C6 | 1.376 (3) | C16—C17 | 1.384 (3) |
| C5—H5 | 0.9500 | C16—H16 | 0.9500 |
| C6—C7 | 1.375 (3) | C17—C18 | 1.377 (3) |
| C6—H6 | 0.9500 | C17—H17 | 0.9500 |
| C8—C9 | 1.480 (3) | C18—C19 | 1.380 (4) |
| C9—H9A | 0.9800 | C19—C20 | 1.388 (3) |
| C9—H9B | 0.9800 | C19—H19 | 0.9500 |
| C9—H9C | 0.9800 | C20—H20 | 0.9500 |
| | | | |
| C18—Br1—O3ⁱ | 153.82 (8) | C14—C10—H10 | 107.4 |
| O2—S1—O3 | 119.56 (9) | C10—C11—C12 | 105.5 (3) |
| O2—S1—C1 | 107.71 (9) | C10—C11—H11A | 110.6 |
| O3—S1—C1 | 109.06 (9) | C12—C11—H11A | 110.6 |
| O2—S1—C15 | 107.74 (9) | C10—C11—H11B | 110.6 |
| O3—S1—C15 | 107.85 (9) | C12—C11—H11B | 110.6 |
| C1—S1—C15 | 103.80 (9) | H11A—C11—H11B | 108.8 |
| C8—O1—C7 | 106.92 (16) | C13—C12—C11 | 106.2 (3) |
| C8—C1—C2 | 107.78 (17) | C13—C12—H12A | 110.5 |
| C8—C1—S1 | 125.88 (16) | C11—C12—H12A | 110.5 |
| C2—C1—S1 | 125.97 (15) | C13—C12—H12B | 110.5 |
| C3—C2—C7 | 119.27 (18) | C11—C12—H12B | 110.5 |
| C3—C2—C1 | 136.45 (18) | H12A—C12—H12B | 108.7 |
| C7—C2—C1 | 104.23 (18) | C12—C13—C14 | 105.3 (3) |
| C2—C3—C4 | 119.00 (19) | C12—C13—H13A | 110.7 |
| C2—C3—H3 | 120.5 | C14—C13—H13A | 110.7 |
| C4—C3—H3 | 120.5 | C12—C13—H13B | 110.7 |
| C3—C4—C5 | 119.2 (2) | C14—C13—H13B | 110.7 |
| C3—C4—C10 | 121.13 (19) | H13A—C13—H13B | 108.8 |
| C5—C4—C10 | 119.70 (18) | C10—C14—C13 | 103.9 (3) |
| C6—C5—C4 | 122.7 (2) | C10—C14—H14A | 111.0 |
| C6—C5—H5 | 118.6 | C13—C14—H14A | 111.0 |
| C4—C5—H5 | 118.6 | C10—C14—H14B | 111.0 |

| | | | |
|---|---|---|---|
| C7—C6—C5 | 116.3 (2) | C13—C14—H14B | 111.0 |
| C7—C6—H6 | 121.9 | H14A—C14—H14B | 109.0 |
| C5—C6—H6 | 121.9 | C16—C15—C20 | 121.06 (19) |
| C6—C7—O1 | 125.68 (19) | C16—C15—S1 | 119.38 (16) |
| C6—C7—C2 | 123.5 (2) | C20—C15—S1 | 119.55 (15) |
| O1—C7—C2 | 110.74 (17) | C17—C16—C15 | 119.4 (2) |
| C1—C8—O1 | 110.30 (18) | C17—C16—H16 | 120.3 |
| C1—C8—C9 | 134.34 (19) | C15—C16—H16 | 120.3 |
| O1—C8—C9 | 115.33 (18) | C18—C17—C16 | 119.2 (2) |
| C8—C9—H9A | 109.5 | C18—C17—H17 | 120.4 |
| C8—C9—H9B | 109.5 | C16—C17—H17 | 120.4 |
| H9A—C9—H9B | 109.5 | C17—C18—C19 | 122.2 (2) |
| C8—C9—H9C | 109.5 | C17—C18—Br1 | 118.42 (18) |
| H9A—C9—H9C | 109.5 | C19—C18—Br1 | 119.40 (18) |
| H9B—C9—H9C | 109.5 | C18—C19—C20 | 118.8 (2) |
| C4—C10—C11 | 116.0 (2) | C18—C19—H19 | 120.6 |
| C4—C10—C14 | 116.3 (2) | C20—C19—H19 | 120.6 |
| C11—C10—C14 | 101.7 (2) | C19—C20—C15 | 119.4 (2) |
| C4—C10—H10 | 107.4 | C19—C20—H20 | 120.3 |
| C11—C10—H10 | 107.4 | C15—C20—H20 | 120.3 |
| | | | |
| O2—S1—C1—C8 | −155.71 (19) | C7—O1—C8—C9 | −176.6 (2) |
| O3—S1—C1—C8 | −24.5 (2) | C3—C4—C10—C11 | 53.8 (3) |
| C15—S1—C1—C8 | 90.2 (2) | C5—C4—C10—C11 | −124.7 (3) |
| O2—S1—C1—C2 | 32.2 (2) | C3—C4—C10—C14 | −65.7 (3) |
| O3—S1—C1—C2 | 163.33 (17) | C5—C4—C10—C14 | 115.8 (3) |
| C15—S1—C1—C2 | −81.9 (2) | C4—C10—C11—C12 | −164.0 (2) |
| C8—C1—C2—C3 | −176.0 (2) | C14—C10—C11—C12 | −36.8 (3) |
| S1—C1—C2—C3 | −2.7 (4) | C10—C11—C12—C13 | 18.2 (3) |
| C8—C1—C2—C7 | 1.1 (2) | C11—C12—C13—C14 | 7.8 (3) |
| S1—C1—C2—C7 | 174.40 (16) | C4—C10—C14—C13 | 168.5 (2) |
| C7—C2—C3—C4 | −1.2 (3) | C11—C10—C14—C13 | 41.6 (3) |
| C1—C2—C3—C4 | 175.6 (2) | C12—C13—C14—C10 | −30.8 (3) |
| C2—C3—C4—C5 | 1.5 (3) | O2—S1—C15—C16 | 153.86 (15) |
| C2—C3—C4—C10 | −177.0 (2) | O3—S1—C15—C16 | 23.52 (18) |
| C3—C4—C5—C6 | −0.4 (4) | C1—S1—C15—C16 | −92.10 (17) |
| C10—C4—C5—C6 | 178.1 (2) | O2—S1—C15—C20 | −27.16 (18) |
| C4—C5—C6—C7 | −1.0 (4) | O3—S1—C15—C20 | −157.50 (15) |
| C5—C6—C7—O1 | −176.3 (2) | C1—S1—C15—C20 | 86.88 (17) |
| C5—C6—C7—C2 | 1.4 (4) | C20—C15—C16—C17 | −0.2 (3) |
| C8—O1—C7—C6 | 177.0 (2) | S1—C15—C16—C17 | 178.79 (16) |
| C8—O1—C7—C2 | −1.0 (2) | C15—C16—C17—C18 | −0.2 (3) |
| C3—C2—C7—C6 | −0.4 (3) | C16—C17—C18—C19 | 0.4 (3) |
| C1—C2—C7—C6 | −178.1 (2) | C16—C17—C18—Br1 | 179.82 (16) |
| C3—C2—C7—O1 | 177.66 (19) | O3[i]—Br1—C18—C17 | −10.6 (3) |
| C1—C2—C7—O1 | −0.1 (2) | O3[i]—Br1—C18—C19 | 168.84 (12) |
| C2—C1—C8—O1 | −1.8 (3) | C17—C18—C19—C20 | −0.2 (3) |
| S1—C1—C8—O1 | −175.07 (15) | Br1—C18—C19—C20 | −179.62 (15) |
| C2—C1—C8—C9 | 176.1 (3) | C18—C19—C20—C15 | −0.2 (3) |

| S1—C1—C8—C9 | 2.8 (4) | C16—C15—C20—C19 | 0.4 (3) |
| C7—O1—C8—C1 | 1.7 (2) | S1—C15—C20—C19 | −178.60 (15) |

Symmetry code: (i) *x*−1, −*y*+1/2, *z*−1/2.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
| --- | --- | --- | --- | --- |
| C17—H17···O2[ii] | 0.95 | 2.51 | 3.169 (3) | 126 |

Symmetry code: (ii) *x*−1, *y*, *z*.