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## Structure Reports

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## 5-Bromo-2,4,6-trimethyl-3-(4-methylphenylsulfanyl)-1-benzofuran

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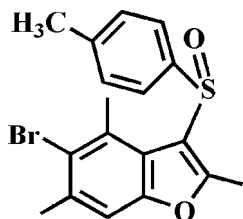
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Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å;  $R$  factor = 0.062;  $wR$  factor = 0.177; data-to-parameter ratio = 14.1.

In the title compound,  $\text{C}_{18}\text{H}_{17}\text{BrO}_2\text{S}$ , the dihedral angle between the methylphenyl ring and the mean plane of the benzofuran ring system is  $87.0(2)^\circ$ . In the crystal, molecules related by inversion are paired into dimers via  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\pi$  interactions. These dimers are further linked by  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds and  $\pi-\pi$  interactions between the benzene and furan rings of neighbouring molecules [centroid-centroid distance =  $3.555(5)$  Å], resulting in a three-dimensional supramolecular network.

## Related literature

For background information and the crystal structures of related compounds, see: Choi *et al.* (2008, 2011).



## Experimental

## Crystal data

 $\text{C}_{18}\text{H}_{17}\text{BrO}_2\text{S}$  $M_r = 377.29$ 

Triclinic,  $P\bar{1}$   
 $a = 8.793(5)$  Å  
 $b = 9.229(5)$  Å  
 $c = 10.861(6)$  Å  
 $\alpha = 86.105(16)^\circ$   
 $\beta = 69.582(17)^\circ$   
 $\gamma = 80.550(16)^\circ$

$V = 814.7(8)$  Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 2.66$  mm<sup>-1</sup>  
 $T = 173$  K  
 $0.42 \times 0.35 \times 0.23$  mm

## Data collection

Bruker SMART APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2009)  
 $T_{\min} = 0.402$ ,  $T_{\max} = 0.580$

10322 measured reflections  
 2857 independent reflections  
 2420 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.067$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$   
 $wR(F^2) = 0.177$   
 $S = 1.15$   
 2857 reflections

203 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 1.44$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.27$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

Cg2 is the centroid of the C1/C2/C7/O1/C8 furan ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C6}-\text{H6}\cdots\text{O2}^i$	0.95	2.32	3.181 (6)	151
$\text{C17}-\text{H17}\cdots\text{O1}^{ii}$	0.95	2.58	3.456 (6)	154
$\text{C11}-\text{H11A}\cdots\text{Cg2}^{ii}$	0.98	2.83	3.794 (6)	167

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

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 for Windows (Farrugia, 2012) and DIAMOND (Brandenburg, 1998); software used to prepare material for publication: SHELXL97.

Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5773).

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## supporting information

*Acta Cryst.* (2014). E70, o381 [doi:10.1107/S1600536814004310]

**5-Bromo-2,4,6-trimethyl-3-(4-methylphenylsulfinyl)-1-benzofuran**

Hong Dae Choi, Pil Ja Seo and Uk Lee

**S1. Comment**

As a part of our continuing study of 5-bromo-2,4,6-trimethyl-1-benzofuran derivatives containing phenylsulfinyl (Choi *et al.*, 2008) and 4-fluorophenylsulfinyl (Choi *et al.*, 2011) substituents in 3-position, we report here the crystal structure of the title compound.

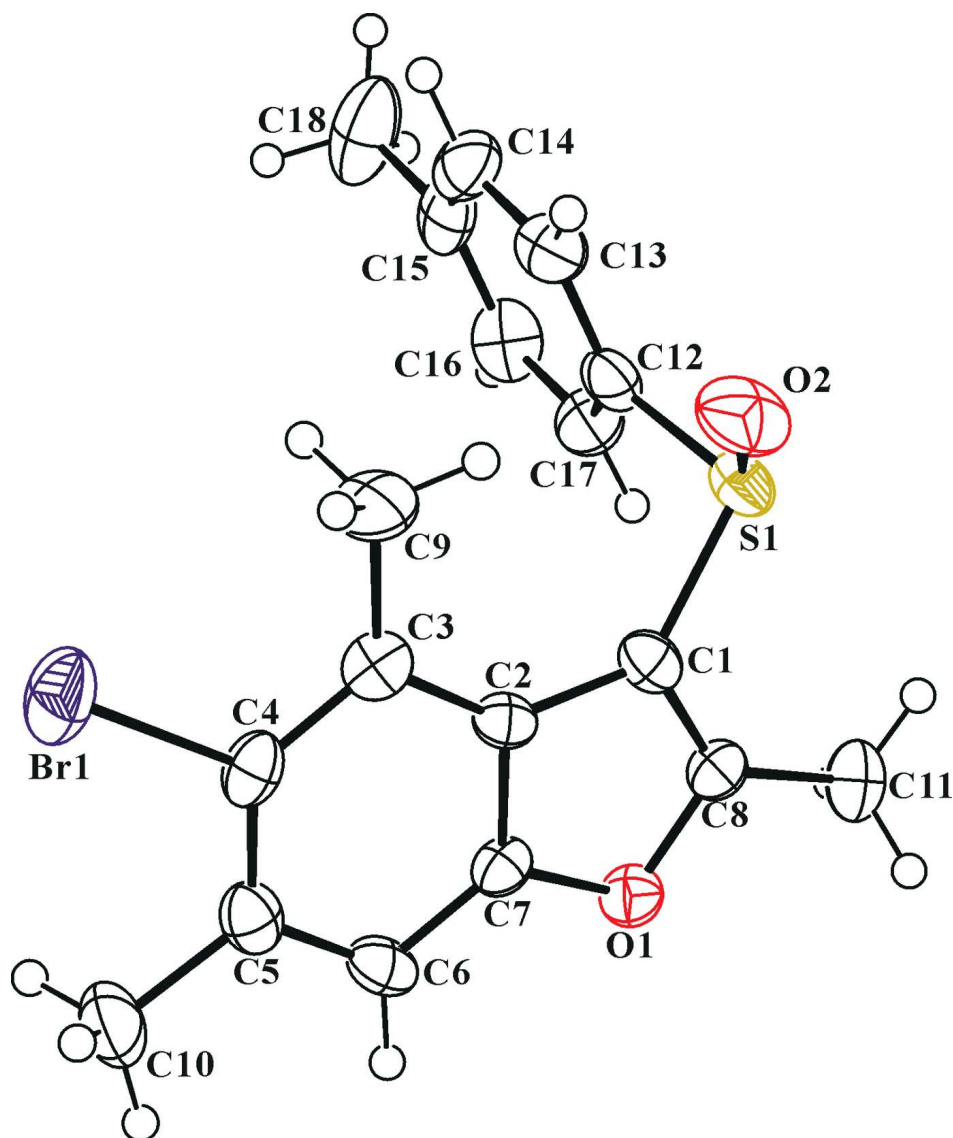
In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.017 (3) Å from the least-squares plane defined by the nine constituent atoms. The 4-methylphenyl ring is essentially planar, with a mean deviation of 0.007 (4) Å from the least-squares plane defined by the six constituent atoms. The dihedral angle formed by the benzofuran ring system and the 4-methylphenyl ring is 87.0 (2)°. In the crystal structure, Fig. 2, the molecules related by inversion are paired into dimers via C—H···O and C—H··· $\pi$  interactions (Table 1, Cg2 is the centroid of the C1/C2/C7/O1/C8 furan ring). These dimers are further packed by intermolecular C—H···O hydrogen bonds (Table 1) and  $\pi$ ··· $\pi$  interactions between the benzene and furan rings of neighbouring molecules, with a Cg1···Cg2<sup>iii</sup> distance of 3.555 (5) Å and an interplanar distance of 3.499 (5) Å resulting in a slippage of 0.629 (5) Å (Cg1 is the centroid of the C2–C7 benzene ring), resulting in a three-dimensional network.

**S2. Experimental**

3-Chloroperoxybenzoic acid (77%, 224 mg, 1.0 mmol) was added in small portions to a stirred solution of 5-bromo-2,4,6-trimethyl-3-(4-methylphenylsulfonyl)-1-benzofuran (325 mg, 0.9 mmol) in dichloromethane (30 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, 2:1 v/v) to afford the title compound as a colorless solid [yield 69%, m.p. 470–471 K;  $R_f$  = 0.51 (hexane–ethyl acetate, 2:1 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.

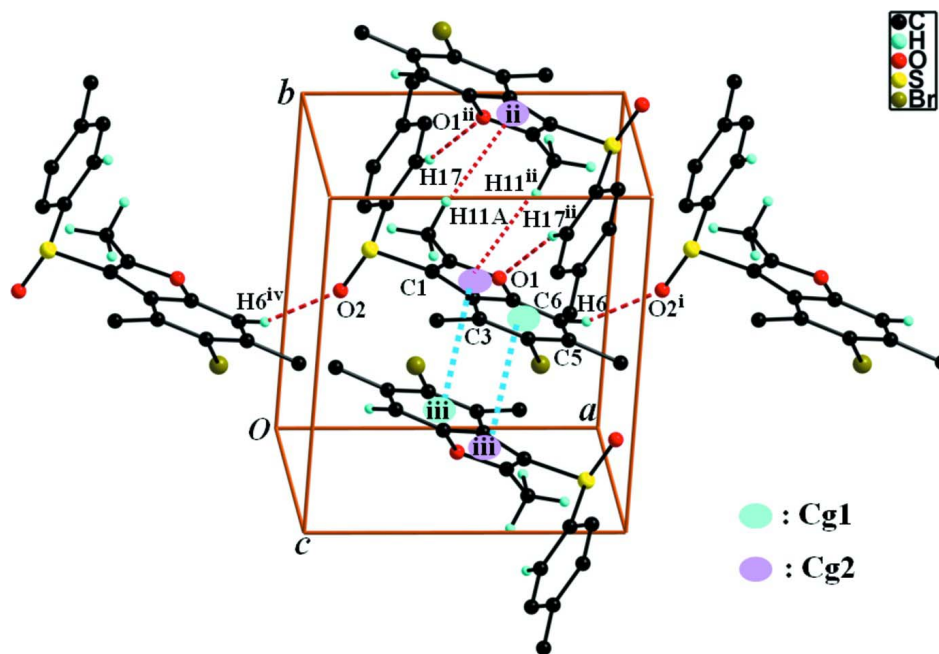
**S3. Refinement**

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.  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aryl and  $1.5U_{\text{eq}}(\text{C})$  for methyl H atoms. The positions of methyl hydrogens were optimized rotationally. The highest peak in the difference map is 0.88 Å from BR1 and the deepest hole is 0.95 Å from BR1.



**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 (dotted lines) in the crystal structure of the title compound. H atoms non-participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i)  $x + 1, y, z$ ; (ii)  $-x + 1, -y + 2, -z + 2$ ; (iii)  $-x + 1, -y + 1, -z + 2$ ; (iv)  $x - 1, y, z$ .]

### 5-Bromo-2,4,6-trimethyl-3-(4-methylphenylsulfinyl)-1-benzofuran

#### Crystal data

$C_{18}H_{17}BrO_2S$

$M_r = 377.29$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 8.793\ (5)\ \text{\AA}$

$b = 9.229\ (5)\ \text{\AA}$

$c = 10.861\ (6)\ \text{\AA}$

$\alpha = 86.105\ (16)^\circ$

$\beta = 69.582\ (17)^\circ$

$\gamma = 80.550\ (16)^\circ$

$V = 814.7\ (8)\ \text{\AA}^3$

$Z = 2$

$F(000) = 384$

$D_x = 1.538\ \text{Mg m}^{-3}$

Melting point = 470–471 K

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

Cell parameters from 5866 reflections

$\theta = 2.2\text{--}28.2^\circ$

$\mu = 2.66\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Block, colourless

$0.42 \times 0.35 \times 0.23\ \text{mm}$

#### Data collection

Bruker SMART APEXII CCD  
diffractometer

Radiation source: rotating anode

Graphite multilayer monochromator

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

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.402, T_{\max} = 0.580$

10322 measured reflections

2857 independent reflections

2420 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.067$

$\theta_{\text{max}} = 25.0^\circ, \theta_{\text{min}} = 2.0^\circ$

$h = -10 \rightarrow 10$

$k = -10 \rightarrow 10$

$l = -12 \rightarrow 12$

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.062$  $wR(F^2) = 0.177$  $S = 1.15$ 

2857 reflections

203 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
map

Hydrogen site location: difference Fourier map

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0949P)^2 + 1.1374P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.001$  $\Delta\rho_{\max} = 1.44 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -1.27 \text{ e } \text{\AA}^{-3}$ *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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.73930 (7)	0.37481 (6)	0.59473 (5)	0.0546 (3)
S1	0.14037 (13)	0.83306 (15)	0.96038 (13)	0.0394 (3)
O1	0.5385 (4)	0.7754 (3)	1.0502 (3)	0.0328 (7)
O2	0.0597 (5)	0.7075 (5)	0.9495 (4)	0.0571 (11)
C1	0.3381 (5)	0.7704 (5)	0.9688 (5)	0.0319 (10)
C2	0.4792 (5)	0.6678 (5)	0.8932 (4)	0.0276 (9)
C3	0.5165 (6)	0.5721 (5)	0.7880 (5)	0.0346 (10)
C4	0.6773 (6)	0.4989 (5)	0.7443 (5)	0.0346 (10)
C5	0.7984 (6)	0.5111 (5)	0.7983 (5)	0.0360 (11)
C6	0.7561 (5)	0.6025 (5)	0.9048 (5)	0.0346 (11)
H6	0.8326	0.6129	0.9463	0.042*
C7	0.5984 (5)	0.6779 (5)	0.9481 (4)	0.0278 (9)
C8	0.3796 (5)	0.8293 (5)	1.0595 (4)	0.0307 (10)
C9	0.3914 (7)	0.5491 (7)	0.7294 (6)	0.0503 (14)
H9A	0.4179	0.5943	0.6416	0.075*
H9B	0.2824	0.5945	0.7855	0.075*
H9C	0.3921	0.4436	0.7229	0.075*
C10	0.9707 (6)	0.4268 (7)	0.7463 (6)	0.0520 (14)
H10A	1.0319	0.4439	0.8028	0.078*
H10B	1.0265	0.4603	0.6566	0.078*
H10C	0.9653	0.3216	0.7459	0.078*
C11	0.2953 (7)	0.9413 (6)	1.1636 (5)	0.0447 (12)
H11A	0.3449	1.0314	1.1384	0.067*
H11B	0.3071	0.9033	1.2468	0.067*
H11C	0.1786	0.9629	1.1742	0.067*

C12	0.1975 (5)	0.9215 (5)	0.8030 (5)	0.0353 (11)
C13	0.1410 (6)	0.8845 (6)	0.7076 (6)	0.0413 (12)
H13	0.0813	0.8043	0.7215	0.050*
C14	0.1720 (7)	0.9653 (6)	0.5911 (5)	0.0450 (12)
H14	0.1340	0.9392	0.5250	0.054*
C15	0.2570 (7)	1.0826 (6)	0.5702 (5)	0.0459 (13)
C16	0.3127 (7)	1.1186 (6)	0.6677 (6)	0.0485 (14)
H16	0.3734	1.1980	0.6538	0.058*
C17	0.2810 (6)	1.0405 (6)	0.7841 (5)	0.0414 (12)
H17	0.3162	1.0681	0.8513	0.050*
C18	0.2899 (11)	1.1726 (8)	0.4462 (6)	0.075 (2)
H18A	0.3956	1.1316	0.3821	0.112*
H18B	0.2933	1.2741	0.4653	0.112*
H18C	0.2025	1.1711	0.4101	0.112*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.0716 (5)	0.0430 (4)	0.0419 (4)	−0.0002 (3)	−0.0117 (3)	−0.0140 (3)
S1	0.0234 (5)	0.0507 (7)	0.0420 (7)	−0.0043 (5)	−0.0094 (5)	0.0013 (6)
O1	0.0333 (16)	0.0353 (17)	0.0331 (18)	−0.0088 (13)	−0.0132 (13)	−0.0042 (14)
O2	0.0391 (19)	0.068 (3)	0.070 (3)	−0.0237 (18)	−0.0217 (19)	0.015 (2)
C1	0.026 (2)	0.031 (2)	0.037 (3)	−0.0052 (17)	−0.0097 (18)	0.0021 (19)
C2	0.026 (2)	0.028 (2)	0.033 (2)	−0.0085 (16)	−0.0128 (17)	0.0018 (18)
C3	0.042 (3)	0.029 (2)	0.036 (3)	−0.0090 (19)	−0.015 (2)	0.001 (2)
C4	0.046 (3)	0.028 (2)	0.028 (2)	−0.0071 (19)	−0.0085 (19)	−0.0049 (18)
C5	0.033 (2)	0.034 (2)	0.036 (3)	−0.0050 (19)	−0.0055 (19)	0.003 (2)
C6	0.024 (2)	0.039 (3)	0.044 (3)	−0.0084 (18)	−0.014 (2)	0.005 (2)
C7	0.031 (2)	0.031 (2)	0.026 (2)	−0.0122 (17)	−0.0111 (17)	−0.0006 (17)
C8	0.034 (2)	0.031 (2)	0.027 (2)	−0.0066 (18)	−0.0106 (18)	0.0022 (18)
C9	0.051 (3)	0.053 (3)	0.059 (4)	−0.006 (2)	−0.032 (3)	−0.018 (3)
C10	0.035 (3)	0.059 (3)	0.048 (3)	0.002 (2)	−0.001 (2)	−0.002 (3)
C11	0.046 (3)	0.044 (3)	0.037 (3)	−0.005 (2)	−0.003 (2)	−0.009 (2)
C12	0.027 (2)	0.034 (2)	0.041 (3)	0.0061 (18)	−0.0106 (19)	−0.005 (2)
C13	0.039 (3)	0.037 (3)	0.050 (3)	−0.004 (2)	−0.018 (2)	−0.006 (2)
C14	0.057 (3)	0.041 (3)	0.037 (3)	0.006 (2)	−0.020 (2)	−0.010 (2)
C15	0.056 (3)	0.032 (3)	0.038 (3)	0.006 (2)	−0.007 (2)	−0.010 (2)
C16	0.053 (3)	0.034 (3)	0.054 (4)	−0.009 (2)	−0.010 (3)	−0.001 (2)
C17	0.044 (3)	0.040 (3)	0.043 (3)	−0.008 (2)	−0.017 (2)	−0.006 (2)
C18	0.111 (6)	0.051 (4)	0.040 (4)	0.001 (4)	−0.006 (4)	0.002 (3)

*Geometric parameters (Å, °)*

Br1—C4	1.918 (5)	C10—H10A	0.9800
S1—O2	1.485 (4)	C10—H10B	0.9800
S1—C1	1.772 (5)	C10—H10C	0.9800
S1—C12	1.785 (5)	C11—H11A	0.9800
O1—C8	1.374 (6)	C11—H11B	0.9800

O1—C7	1.375 (6)	C11—H11C	0.9800
C1—C8	1.337 (7)	C12—C13	1.378 (8)
C1—C2	1.456 (6)	C12—C17	1.384 (7)
C2—C7	1.392 (6)	C13—C14	1.389 (8)
C2—C3	1.405 (7)	C13—H13	0.9500
C3—C4	1.393 (7)	C14—C15	1.378 (8)
C3—C9	1.497 (7)	C14—H14	0.9500
C4—C5	1.406 (7)	C15—C16	1.391 (9)
C5—C6	1.384 (7)	C15—C18	1.497 (8)
C5—C10	1.515 (7)	C16—C17	1.375 (8)
C6—C7	1.378 (6)	C16—H16	0.9500
C6—H6	0.9500	C17—H17	0.9500
C8—C11	1.490 (7)	C18—H18A	0.9800
C9—H9A	0.9800	C18—H18B	0.9800
C9—H9B	0.9800	C18—H18C	0.9800
C9—H9C	0.9800		
O2—S1—C1	110.8 (2)	C5—C10—H10B	109.5
O2—S1—C12	106.7 (2)	H10A—C10—H10B	109.5
C1—S1—C12	99.4 (2)	C5—C10—H10C	109.5
C8—O1—C7	106.3 (3)	H10A—C10—H10C	109.5
C8—C1—C2	107.6 (4)	H10B—C10—H10C	109.5
C8—C1—S1	117.8 (4)	C8—C11—H11A	109.5
C2—C1—S1	134.5 (4)	C8—C11—H11B	109.5
C7—C2—C3	119.4 (4)	H11A—C11—H11B	109.5
C7—C2—C1	104.1 (4)	C8—C11—H11C	109.5
C3—C2—C1	136.6 (4)	H11A—C11—H11C	109.5
C4—C3—C2	114.9 (4)	H11B—C11—H11C	109.5
C4—C3—C9	122.9 (5)	C13—C12—C17	120.2 (5)
C2—C3—C9	122.2 (4)	C13—C12—S1	120.4 (4)
C3—C4—C5	125.7 (4)	C17—C12—S1	118.8 (4)
C3—C4—Br1	116.9 (4)	C12—C13—C14	119.5 (5)
C5—C4—Br1	117.4 (4)	C12—C13—H13	120.2
C6—C5—C4	118.0 (4)	C14—C13—H13	120.2
C6—C5—C10	119.3 (5)	C15—C14—C13	120.9 (5)
C4—C5—C10	122.7 (5)	C15—C14—H14	119.6
C7—C6—C5	117.2 (4)	C13—C14—H14	119.6
C7—C6—H6	121.4	C14—C15—C16	118.8 (5)
C5—C6—H6	121.4	C14—C15—C18	121.9 (6)
O1—C7—C6	124.4 (4)	C16—C15—C18	119.3 (6)
O1—C7—C2	110.8 (4)	C17—C16—C15	120.8 (5)
C6—C7—C2	124.8 (4)	C17—C16—H16	119.6
C1—C8—O1	111.2 (4)	C15—C16—H16	119.6
C1—C8—C11	134.7 (5)	C16—C17—C12	119.8 (5)
O1—C8—C11	114.0 (4)	C16—C17—H17	120.1
C3—C9—H9A	109.5	C12—C17—H17	120.1
C3—C9—H9B	109.5	C15—C18—H18A	109.5
H9A—C9—H9B	109.5	C15—C18—H18B	109.5

C3—C9—H9C	109.5	H18A—C18—H18B	109.5
H9A—C9—H9C	109.5	C15—C18—H18C	109.5
H9B—C9—H9C	109.5	H18A—C18—H18C	109.5
C5—C10—H10A	109.5	H18B—C18—H18C	109.5
O2—S1—C1—C8	-134.4 (4)	C5—C6—C7—C2	0.5 (7)
C12—S1—C1—C8	113.6 (4)	C3—C2—C7—O1	-179.3 (4)
O2—S1—C1—C2	48.7 (5)	C1—C2—C7—O1	1.0 (5)
C12—S1—C1—C2	-63.3 (5)	C3—C2—C7—C6	1.7 (7)
C8—C1—C2—C7	-0.9 (5)	C1—C2—C7—C6	-178.0 (4)
S1—C1—C2—C7	176.2 (4)	C2—C1—C8—O1	0.6 (5)
C8—C1—C2—C3	179.5 (5)	S1—C1—C8—O1	-177.1 (3)
S1—C1—C2—C3	-3.4 (8)	C2—C1—C8—C11	178.4 (5)
C7—C2—C3—C4	-2.6 (6)	S1—C1—C8—C11	0.7 (7)
C1—C2—C3—C4	177.0 (5)	C7—O1—C8—C1	0.0 (5)
C7—C2—C3—C9	176.4 (5)	C7—O1—C8—C11	-178.3 (4)
C1—C2—C3—C9	-4.1 (8)	O2—S1—C12—C13	10.6 (4)
C2—C3—C4—C5	1.6 (7)	C1—S1—C12—C13	125.8 (4)
C9—C3—C4—C5	-177.3 (5)	O2—S1—C12—C17	-177.8 (4)
C2—C3—C4—Br1	-176.7 (3)	C1—S1—C12—C17	-62.6 (4)
C9—C3—C4—Br1	4.4 (6)	C17—C12—C13—C14	1.6 (7)
C3—C4—C5—C6	0.5 (7)	S1—C12—C13—C14	173.0 (4)
Br1—C4—C5—C6	178.8 (3)	C12—C13—C14—C15	-0.6 (8)
C3—C4—C5—C10	179.4 (5)	C13—C14—C15—C16	0.4 (8)
Br1—C4—C5—C10	-2.3 (6)	C13—C14—C15—C18	-179.2 (5)
C4—C5—C6—C7	-1.5 (6)	C14—C15—C16—C17	-1.3 (8)
C10—C5—C6—C7	179.5 (4)	C18—C15—C16—C17	178.4 (5)
C8—O1—C7—C6	178.3 (4)	C15—C16—C17—C12	2.2 (8)
C8—O1—C7—C2	-0.7 (4)	C13—C12—C17—C16	-2.4 (7)
C5—C6—C7—O1	-178.3 (4)	S1—C12—C17—C16	-174.0 (4)

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

Cg2 is the centroid of the C1/C2/C7/O1/C8 furan ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6—H6 $\cdots$ O2 <sup>i</sup>	0.95	2.32	3.181 (6)	151
C17—H17 $\cdots$ O1 <sup>ii</sup>	0.95	2.58	3.456 (6)	154
C11—H11A $\cdots$ Cg2 <sup>ii</sup>	0.98	2.83	3.794 (6)	167

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