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2,5,7-Trimethyl-3-(4-methylphenylsulfonyl)-1-benzofuran

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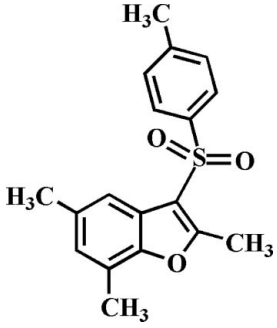
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.116; data-to-parameter ratio = 19.1.

In the title compound, $C_{18}H_{18}O_3S$, the 4-methylphenyl ring makes a dihedral angle of 86.35 (3)° with the mean plane [mean deviation = 0.006 (1) Å] of the benzofuran fragment. In the crystal, molecules are linked by weak C—H···O and C—H···π interactions. The crystal structure also exhibits weak π–π interactions between the furan and benzene rings of neighbouring benzofuran systems [centroid–centroid distance = 3.685 (2), interplanar distance = 3.572 (2) and slippage = 0.906 (2) Å].

Related literature

For background information and the crystal structures of related compounds, see: Choi *et al.* (2008, 2010); Seo *et al.* (2011).



Experimental

Crystal data

$C_{18}H_{18}O_3S$
M_r = 314.38
Monoclinic, $P2_1/c$
a = 9.7666 (2) Å
b = 19.4511 (5) Å
c = 8.2979 (2) Å
β = 98.541 (1)°
V = 1558.88 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 173 K
0.41 × 0.39 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.916, T_{max} = 0.958
15446 measured reflections
3868 independent reflections
3258 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.116
S = 1.04
3868 reflections
203 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C12–C17 benzene ring and the C1/C2/C7/O1/C8 furan ring, respectively

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10*C*···O3^{i}	0.98	2.46	3.310 (2)	146
C9—H9*C*···*Cg*1^{ii}	0.98	2.93	3.907 (2)	179
C10—H10*B*···*Cg*2^{iii}	0.98	2.92	3.800 (2)	150

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

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: SJ5234).

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supporting information

Acta Cryst. (2012). E**68**, o1751 [doi:10.1107/S160053681202020X]

2,5,7-Trimethyl-3-(4-methylphenylsulfonyl)-1-benzofuran

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S1. Comment

As a part of our ongoing study of 2,5,7-trimethyl-1-benzofuran derivatives containing 3-phenylsulfonyl (Choi *et al.*, 2008), 3-(4-fluorophenylsulfonyl) (Choi *et al.*, 2010) and 3-(3-fluorophenylsulfonyl) (Seo *et al.*, 2011) substituents, 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 (1) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle between the 4-methylphenyl ring and the mean plane of the benzofuran fragment is 86.35 (3)°. In the crystal structure (Fig. 2), molecules are connected by weak intermolecular C—H···O and C—H···π interactions (Table 1). The crystal packing (Fig. 2) also exhibits weak π···π interactions between the furan and benzene rings of neighbouring benzofuran systems, with a Cg2···Cg3^{i} distance of 3.685 (2) Å and an interplanar distance of 3.572 (2) Å resulting in a slippage of 0.906 (2) Å (Cg3 is the centroid of the C2–C7 benzene ring).

S2. Experimental

3-Chloroperoxybenzoic acid (77%, 560 mg, 2.5 mmol) was added in small portions to a stirred solution of 2,5,7-trimethyl-3-(4-methylphenylsulfanyl)-1-benzofuran (338 mg, 1.2 mmol) in dichloromethane (30 mL) at 273 K. After being stirred at room temperature for 10h, 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 78%, m.p. 413–414 K; R_f = 0.48 (hexane–ethyl acetate, 4:1 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. Uiso(H) = 1.2U_{eq}(C) for aryl and 1.5U_{eq}(C) for methyl H atoms. The positions of methyl hydrogens were optimized rotationally.

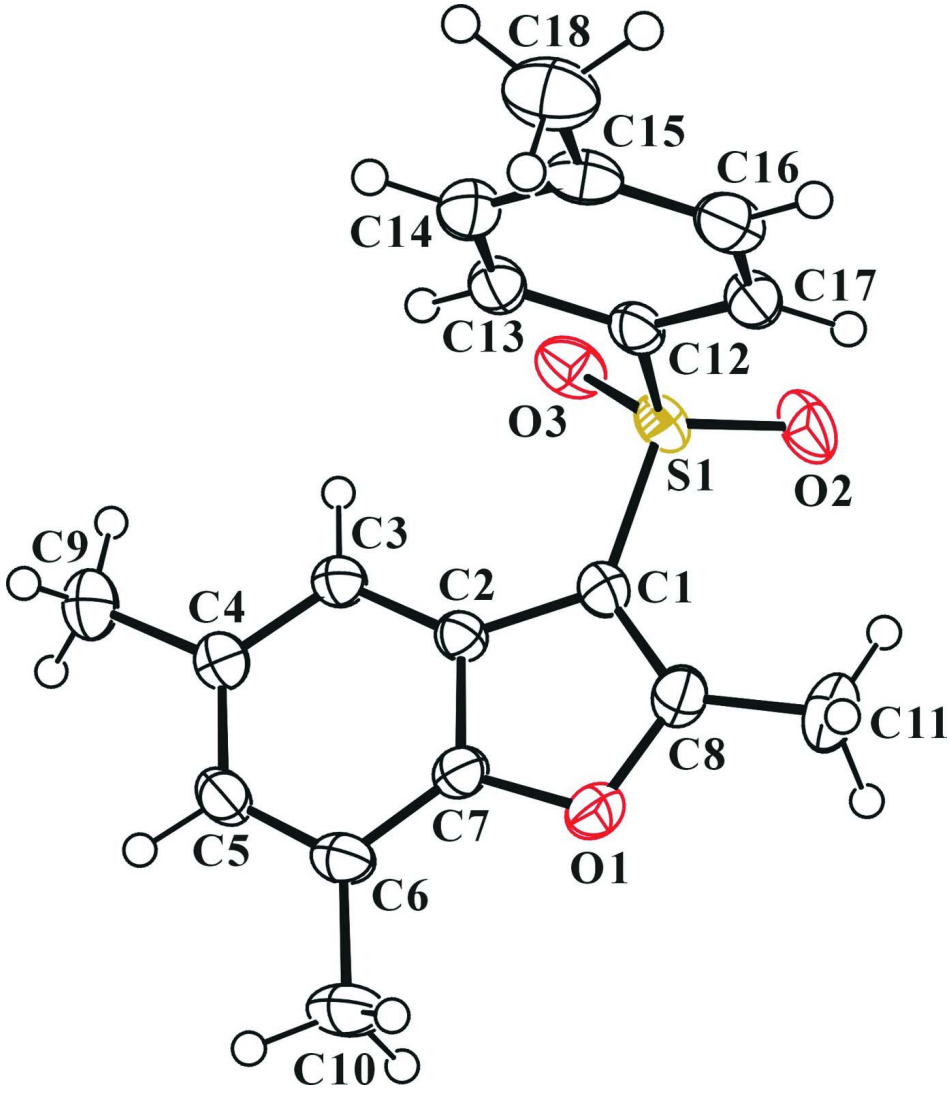

Figure 1

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.

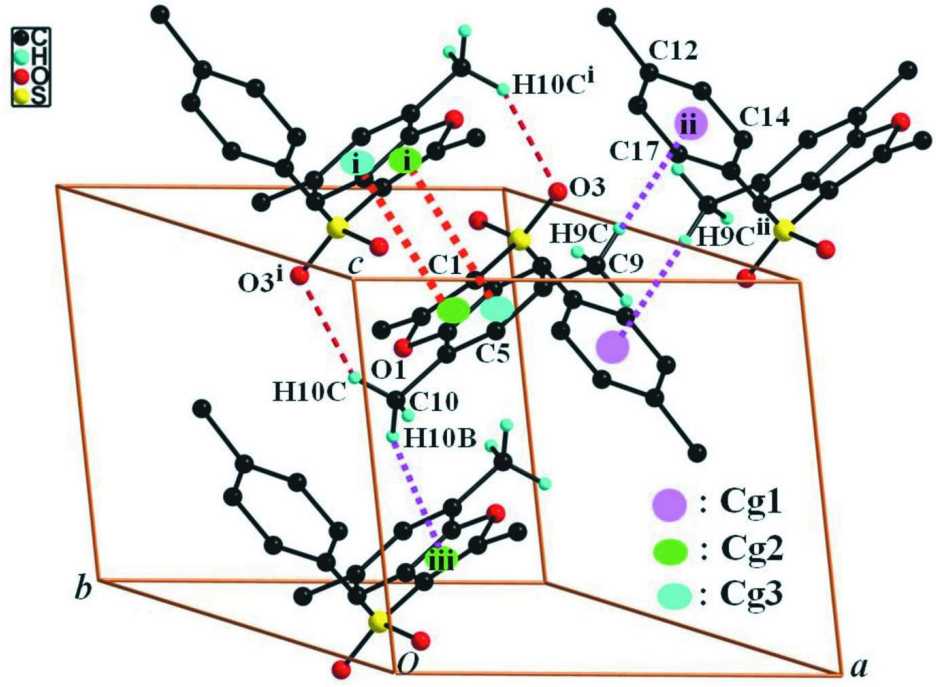

Figure 2

A view of the C—H···O, C—H···π and π···π 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 + 1, - z + 2; (ii) - x + 2, - y + 1, - z + 2; (iii) - x + 1, - y + 1, - z + 1.]

2,5,7-Trimethyl-3-(4-methylphenylsulfonyl)-1-benzofuran

Crystal data

$C_{18}H_{18}O_3S$
M_r = 314.38
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 9.7666 (2) Å
b = 19.4511 (5) Å
c = 8.2979 (2) Å
β = 98.541 (1)°
V = 1558.88 (6) Å^3
Z = 4
$F(000)$ = 664
D_x = 1.340 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5168 reflections
θ = 2.4–28.2°
μ = 0.22 mm^{-1}
T = 173 K
Block, colourless
0.41 × 0.39 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: rotating anode
Graphite multilayer monochromator
Detector resolution: 10.0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.916, T_{max} = 0.958
15446 measured reflections
3868 independent reflections
3258 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 28.4°, θ_{min} = 2.1°
h = −13→12
k = −21→25
l = −11→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.116$
$S = 1.04$
3868 reflections
203 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.5651P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.77821 (4)	0.617621 (19)	0.95912 (5)	0.03124 (12)
O1	0.44316 (10)	0.54239 (6)	0.69953 (13)	0.0335 (3)
O2	0.73376 (14)	0.68604 (6)	0.99116 (16)	0.0445 (3)
O3	0.84855 (13)	0.57685 (6)	1.09059 (14)	0.0401 (3)
C1	0.63766 (15)	0.56994 (7)	0.86672 (18)	0.0281 (3)
C2	0.62873 (14)	0.49571 (7)	0.86149 (17)	0.0259 (3)
C3	0.70807 (15)	0.44093 (8)	0.93316 (18)	0.0295 (3)
H3	0.7907	0.4490	1.0067	0.035*
C4	0.66347 (16)	0.37470 (8)	0.8946 (2)	0.0328 (3)
C5	0.54034 (16)	0.36373 (8)	0.7862 (2)	0.0342 (3)
H5	0.5122	0.3177	0.7612	0.041*
C6	0.45823 (15)	0.41655 (9)	0.71436 (19)	0.0321 (3)
C7	0.50737 (14)	0.48180 (8)	0.75612 (18)	0.0276 (3)
C8	0.52485 (16)	0.59479 (8)	0.7677 (2)	0.0329 (3)
C9	0.7482 (2)	0.31384 (9)	0.9655 (3)	0.0463 (4)
H9A	0.7937	0.2924	0.8806	0.069*
H9B	0.6873	0.2803	1.0071	0.069*
H9C	0.8185	0.3294	1.0547	0.069*
C10	0.32615 (17)	0.40458 (11)	0.5996 (2)	0.0438 (4)
H10A	0.3180	0.3557	0.5713	0.066*
H10B	0.3273	0.4318	0.5003	0.066*
H10C	0.2471	0.4185	0.6522	0.066*
C11	0.4770 (2)	0.66466 (10)	0.7171 (3)	0.0498 (5)
H11A	0.4870	0.6718	0.6026	0.075*
H11B	0.5328	0.6987	0.7849	0.075*

H11C	0.3795	0.6698	0.7305	0.075*
C12	0.88605 (15)	0.62242 (7)	0.80711 (18)	0.0281 (3)
C15	1.04793 (16)	0.62512 (9)	0.55823 (19)	0.0355 (4)
C16	0.97063 (16)	0.68243 (9)	0.5909 (2)	0.0360 (4)
H16	0.9738	0.7228	0.5273	0.043*
C17	0.88939 (16)	0.68161 (8)	0.71428 (19)	0.0323 (3)
H17	0.8369	0.7209	0.7350	0.039*
C18	1.1300 (2)	0.62519 (11)	0.4184 (2)	0.0504 (5)
H18A	1.0714	0.6089	0.3196	0.076*
H18B	1.2102	0.5948	0.4439	0.076*
H18C	1.1617	0.6720	0.4006	0.076*
C13	0.96346 (15)	0.56489 (8)	0.77825 (19)	0.0317 (3)
H13	0.9609	0.5247	0.8426	0.038*
C14	1.04408 (16)	0.56690 (8)	0.6550 (2)	0.0355 (3)
H14	1.0979	0.5279	0.6359	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0373 (2)	0.0257 (2)	0.0299 (2)	−0.00632 (14)	0.00250 (15)	−0.00488 (14)
O1	0.0277 (5)	0.0347 (6)	0.0360 (6)	0.0051 (4)	−0.0020 (4)	−0.0004 (5)
O2	0.0568 (7)	0.0282 (6)	0.0508 (7)	−0.0068 (5)	0.0156 (6)	−0.0142 (5)
O3	0.0457 (6)	0.0439 (7)	0.0279 (6)	−0.0111 (5)	−0.0041 (5)	0.0011 (5)
C1	0.0300 (7)	0.0248 (7)	0.0295 (7)	−0.0007 (5)	0.0039 (6)	−0.0024 (6)
C2	0.0259 (6)	0.0257 (7)	0.0256 (7)	−0.0019 (5)	0.0022 (5)	−0.0022 (5)
C3	0.0268 (6)	0.0281 (7)	0.0321 (8)	−0.0014 (5)	−0.0005 (5)	0.0012 (6)
C4	0.0333 (7)	0.0275 (8)	0.0373 (8)	−0.0011 (6)	0.0046 (6)	0.0016 (6)
C5	0.0350 (8)	0.0270 (7)	0.0410 (9)	−0.0067 (6)	0.0072 (6)	−0.0072 (6)
C6	0.0263 (7)	0.0385 (9)	0.0314 (8)	−0.0060 (6)	0.0040 (6)	−0.0091 (6)
C7	0.0242 (6)	0.0306 (7)	0.0273 (7)	0.0022 (5)	0.0016 (5)	−0.0013 (6)
C8	0.0334 (7)	0.0299 (8)	0.0355 (8)	0.0045 (6)	0.0051 (6)	−0.0001 (6)
C9	0.0503 (10)	0.0282 (9)	0.0590 (12)	0.0037 (7)	0.0032 (8)	0.0053 (8)
C10	0.0293 (7)	0.0596 (11)	0.0405 (9)	−0.0081 (7)	−0.0009 (7)	−0.0155 (8)
C11	0.0514 (10)	0.0350 (9)	0.0611 (12)	0.0153 (8)	0.0022 (9)	0.0067 (9)
C12	0.0283 (7)	0.0251 (7)	0.0287 (7)	−0.0043 (5)	−0.0030 (5)	−0.0012 (6)
C15	0.0278 (7)	0.0457 (9)	0.0311 (8)	−0.0095 (6)	−0.0021 (6)	−0.0032 (7)
C16	0.0346 (8)	0.0359 (8)	0.0349 (8)	−0.0085 (6)	−0.0028 (6)	0.0068 (7)
C17	0.0312 (7)	0.0262 (7)	0.0375 (8)	−0.0023 (6)	−0.0018 (6)	0.0019 (6)
C18	0.0444 (10)	0.0665 (13)	0.0418 (10)	−0.0132 (9)	0.0108 (8)	−0.0055 (9)
C13	0.0313 (7)	0.0272 (7)	0.0342 (8)	−0.0014 (5)	−0.0033 (6)	0.0018 (6)
C14	0.0305 (7)	0.0343 (8)	0.0400 (9)	0.0008 (6)	−0.0008 (6)	−0.0046 (7)

Geometric parameters (Å, º)

S1—O2	1.4369 (12)	C9—H9C	0.9800
S1—O3	1.4382 (12)	C10—H10A	0.9800
S1—C1	1.7377 (15)	C10—H10B	0.9800
S1—C12	1.7617 (16)	C10—H10C	0.9800

O1—C8	1.3643 (19)	C11—H11A	0.9800
O1—C7	1.3840 (17)	C11—H11B	0.9800
C1—C8	1.361 (2)	C11—H11C	0.9800
C1—C2	1.447 (2)	C12—C17	1.388 (2)
C2—C7	1.3909 (19)	C12—C13	1.391 (2)
C2—C3	1.397 (2)	C15—C14	1.392 (2)
C3—C4	1.382 (2)	C15—C16	1.395 (2)
C3—H3	0.9500	C15—C18	1.505 (2)
C4—C5	1.407 (2)	C16—C17	1.385 (2)
C4—C9	1.513 (2)	C16—H16	0.9500
C5—C6	1.383 (2)	C17—H17	0.9500
C5—H5	0.9500	C18—H18A	0.9800
C6—C7	1.383 (2)	C18—H18B	0.9800
C6—C10	1.504 (2)	C18—H18C	0.9800
C8—C11	1.478 (2)	C13—C14	1.381 (2)
C9—H9A	0.9800	C13—H13	0.9500
C9—H9B	0.9800	C14—H14	0.9500

O2—S1—O3	119.59 (8)	C6—C10—H10A	109.5
O2—S1—C1	109.59 (7)	C6—C10—H10B	109.5
O3—S1—C1	107.30 (7)	H10A—C10—H10B	109.5
O2—S1—C12	108.21 (7)	C6—C10—H10C	109.5
O3—S1—C12	107.66 (7)	H10A—C10—H10C	109.5
C1—S1—C12	103.27 (7)	H10B—C10—H10C	109.5
C8—O1—C7	106.73 (11)	C8—C11—H11A	109.5
C8—C1—C2	107.24 (13)	C8—C11—H11B	109.5
C8—C1—S1	126.32 (12)	H11A—C11—H11B	109.5
C2—C1—S1	125.87 (11)	C8—C11—H11C	109.5
C7—C2—C3	119.08 (13)	H11A—C11—H11C	109.5
C7—C2—C1	104.77 (12)	H11B—C11—H11C	109.5
C3—C2—C1	136.15 (13)	C17—C12—C13	120.90 (15)
C4—C3—C2	118.45 (13)	C17—C12—S1	120.47 (12)
C4—C3—H3	120.8	C13—C12—S1	118.59 (11)
C2—C3—H3	120.8	C14—C15—C16	118.43 (15)
C3—C4—C5	119.97 (14)	C14—C15—C18	120.57 (16)
C3—C4—C9	120.27 (15)	C16—C15—C18	120.97 (16)
C5—C4—C9	119.75 (15)	C17—C16—C15	121.36 (15)
C6—C5—C4	123.28 (14)	C17—C16—H16	119.3
C6—C5—H5	118.4	C15—C16—H16	119.3
C4—C5—H5	118.4	C16—C17—C12	118.87 (15)
C7—C6—C5	114.61 (13)	C16—C17—H17	120.6
C7—C6—C10	122.29 (16)	C12—C17—H17	120.6
C5—C6—C10	123.10 (15)	C15—C18—H18A	109.5
C6—C7—O1	125.01 (13)	C15—C18—H18B	109.5
C6—C7—C2	124.59 (14)	H18A—C18—H18B	109.5
O1—C7—C2	110.40 (13)	C15—C18—H18C	109.5
C1—C8—O1	110.86 (13)	H18A—C18—H18C	109.5
C1—C8—C11	133.75 (16)	H18B—C18—H18C	109.5

O1—C8—C11	115.37 (14)	C14—C13—C12	119.27 (14)
C4—C9—H9A	109.5	C14—C13—H13	120.4
C4—C9—H9B	109.5	C12—C13—H13	120.4
H9A—C9—H9B	109.5	C13—C14—C15	121.17 (15)
C4—C9—H9C	109.5	C13—C14—H14	119.4
H9A—C9—H9C	109.5	C15—C14—H14	119.4
H9B—C9—H9C	109.5		

O2—S1—C1—C8	30.29 (16)	C1—C2—C7—C6	179.59 (14)
O3—S1—C1—C8	161.58 (14)	C3—C2—C7—O1	179.33 (13)
C12—S1—C1—C8	−84.84 (15)	C1—C2—C7—O1	−0.47 (16)
O2—S1—C1—C2	−159.46 (13)	C2—C1—C8—O1	0.35 (17)
O3—S1—C1—C2	−28.17 (15)	S1—C1—C8—O1	172.09 (11)
C12—S1—C1—C2	85.40 (14)	C2—C1—C8—C11	−177.50 (19)
C8—C1—C2—C7	0.08 (16)	S1—C1—C8—C11	−5.8 (3)
S1—C1—C2—C7	−171.71 (11)	C7—O1—C8—C1	−0.64 (17)
C8—C1—C2—C3	−179.68 (17)	C7—O1—C8—C11	177.64 (14)
S1—C1—C2—C3	8.5 (3)	O2—S1—C12—C17	−14.89 (14)
C7—C2—C3—C4	0.8 (2)	O3—S1—C12—C17	−145.45 (12)
C1—C2—C3—C4	−179.43 (16)	C1—S1—C12—C17	101.24 (13)
C2—C3—C4—C5	−0.4 (2)	O2—S1—C12—C13	167.49 (12)
C2—C3—C4—C9	178.24 (15)	O3—S1—C12—C13	36.93 (13)
C3—C4—C5—C6	−0.4 (3)	C1—S1—C12—C13	−76.38 (13)
C9—C4—C5—C6	−179.01 (16)	C14—C15—C16—C17	−1.3 (2)
C4—C5—C6—C7	0.6 (2)	C18—C15—C16—C17	176.77 (15)
C4—C5—C6—C10	−179.54 (16)	C15—C16—C17—C12	0.3 (2)
C5—C6—C7—O1	179.95 (14)	C13—C12—C17—C16	0.5 (2)
C10—C6—C7—O1	0.1 (2)	S1—C12—C17—C16	−177.10 (11)
C5—C6—C7—C2	−0.1 (2)	C17—C12—C13—C14	−0.3 (2)
C10—C6—C7—C2	−179.97 (15)	S1—C12—C13—C14	177.35 (11)
C8—O1—C7—C6	−179.37 (15)	C12—C13—C14—C15	−0.7 (2)
C8—O1—C7—C2	0.69 (16)	C16—C15—C14—C13	1.5 (2)
C3—C2—C7—C6	−0.6 (2)	C18—C15—C14—C13	−176.57 (14)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C12–C17 benzene ring and the C1/C2/C7/O1/C8 furan ring, respectively

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*C*···O3^{i}	0.98	2.46	3.310 (2)	146
C9—H9*C*···*Cg*1^{ii}	0.98	2.93	3.907 (2)	179
C10—H10*B*···*Cg*2^{iii}	0.98	2.92	3.800 (2)	150

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (ii) −*x*+2, −*y*+1, −*z*+2; (iii) −*x*+1, −*y*+1, −*z*+1.