

Crystal structure of 2,5-dimethyl-3-(3-methylphenylsulfonyl)-1-benzofuran

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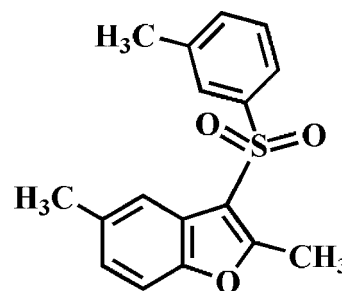
In the title compound, C₁₇H₁₆O₃S, the dihedral angle between the plane of the benzofuran ring system [r.m.s. deviation = 0.010 (1) Å] and that of the 3-methylphenyl ring is 79.09 (5)°. Intramolecular C—H···O hydrogen bonds are observed. In the crystal, molecules are connected into a chain along the *c*-axis direction by two different pairs of inversion-generated interactions: C—H···π hydrogen bonds between the methyl groups and the benzene rings of the 3-methylphenyl fragments and π–π interactions between the benzene and furan rings of neighbouring molecules [centroid–centroid distance = 3.673 (2) Å].

Keywords: crystal structure; benzofuran; 3-methylphenyl; C—H···π hydrogen bonds; π–π interactions.

CCDC reference: 1021292

1. Related literature

For the pharmacological properties of compounds containing a benzofuran moiety, see: Aslam *et al.* (2009); Galal *et al.* (2009); Howlett *et al.* (1999); Khan *et al.* (2005); Ono *et al.* (2002). For natural products with a benzofuran ring, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For the synthesis of the starting material, 2,5-dimethyl-3-(3-methylphenylsulfonyl)-1-benzofuran, see: Choi *et al.* (1999). For a related structure, see: Choi *et al.* (2013).



2. Experimental

2.1. Crystal data

C ₁₇ H ₁₆ O ₃ S	<i>V</i> = 1436.29 (4) Å ³
<i>M_r</i> = 300.36	<i>Z</i> = 4
Monoclinic, <i>P</i> 2 ₁ / <i>n</i>	Mo <i>K</i> α radiation
<i>a</i> = 9.8769 (2) Å	<i>μ</i> = 0.23 mm ⁻¹
<i>b</i> = 11.3190 (2) Å	<i>T</i> = 173 K
<i>c</i> = 13.1320 (2) Å	0.33 × 0.29 × 0.23 mm
<i>β</i> = 101.951 (1)°	

2.2. Data collection

Bruker SMART APEXII CCD diffractometer	13810 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2009)	3589 independent reflections
<i>T_{min}</i> = 0.927, <i>T_{max}</i> = 0.947	2861 reflections with <i>I</i> > 2σ(<i>I</i>)
	<i>R_{int}</i> = 0.035

2.3. Refinement

<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.045	193 parameters
<i>wR</i> (<i>F</i> ²) = 0.128	H-atom parameters constrained
<i>S</i> = 1.08	Δρ _{max} = 0.35 e Å ⁻³
3589 reflections	Δρ _{min} = -0.39 e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C11–C16 3-methylphenyl ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C10—H10C···O3	0.98	2.34	3.078 (3)	131
C17—H17B···Cg1 ⁱ	0.98	2.88	3.478 (2)	121

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

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

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: FY2118).

References

- Akgul, Y. Y. & Anil, H. (2003). *Phytochemistry*, **63**, 939–943.
- Aslam, S. N., Stevenson, P. C., Kokubun, T. & Hall, D. R. (2009). *Microbiol. Res.* **164**, 191–195.
- Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2009). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Choi, H. D., Seo, P. J. & Lee, U. (2013). *Acta Cryst.* **E69**, o817.
- Choi, H. D., Seo, P. J. & Son, B. W. (1999). *J. Korean Chem. Soc.* **43**, 606–608.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Galal, S. A., Abd El-All, A. S., Abdallah, M. M. & El-Diwani, H. I. (2009). *Bioorg. Med. Chem. Lett.* **19**, 2420–2428.
- Howlett, D. R., Perry, A. E., Godfrey, F., Swatton, J. E., Jennings, K. H., Spitzfaden, C., Wadsworth, H., Wood, S. J. & Markwell, R. E. (1999). *Biochem. J.* **340**, 283–289.
- Khan, M. W., Alam, M. J., Rashid, M. A. & Chowdhury, R. (2005). *Bioorg. Med. Chem.* **13**, 4796–4805.
- Ono, M., Kung, M. P., Hou, C. & Kung, H. F. (2002). *Nucl. Med. Biol.* **29**, 633–642.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Soekamto, N. H., Achmad, S. A., Ghisalberti, E. L., Hakim, E. H. & Syah, Y. M. (2003). *Phytochemistry*, **64**, 831–834.

supporting information

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Crystal structure of 2,5-dimethyl-3-(3-methylphenylsulfonyl)-1-benzofuran

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S1. Comment

Molecules containing a benzofuran ring show interesting pharmacological properties such as antibacterial and antifungal, antitumor and antiviral, antimicrobial activities (Aslam *et al.* 2009, Galal *et al.*, 2009, Khan *et al.*, 2005), and they are potential inhibitors of β -amyloid aggregation (Howlett *et al.*, 1999, Ono *et al.*, 2002). These benzofuran compounds are widely occurring in nature (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing program of 3-aryl-sulfonyl-2,5-dimethyl-1-benzofuran derivatives containing 4-methylphenylsulfonyl substituent in 3-position (Choi *et al.*, 2013), we report herein on the crystal structure of the title compound.

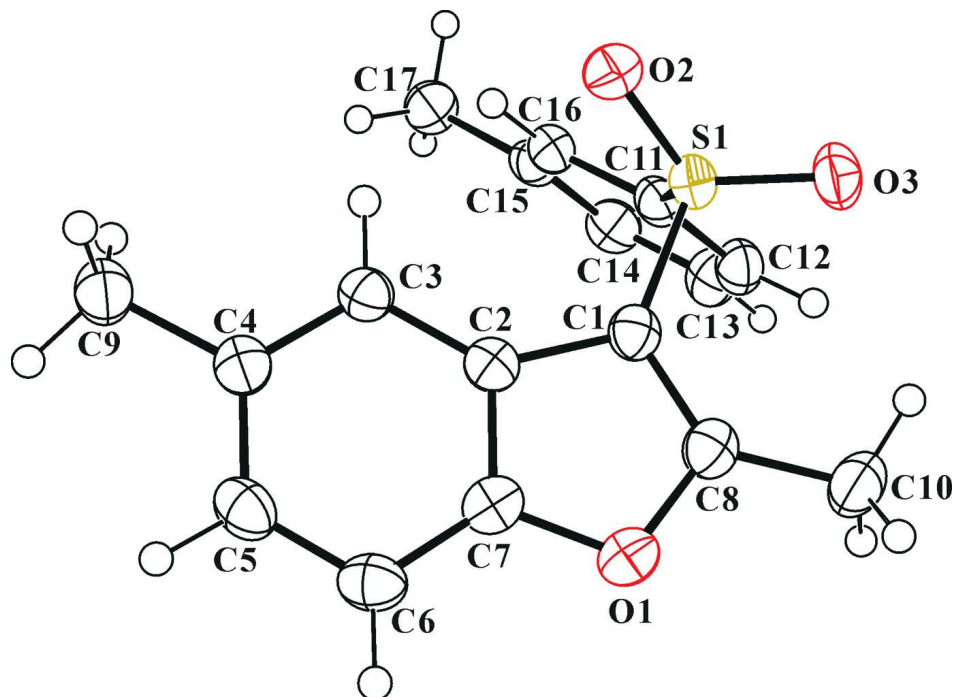
In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.010 (1) Å from the least-squares plane defined by the nine constituent atoms. The 3-methylphenyl ring is essentially planar, with a mean deviation of 0.005 (1) Å from the least-squares plane defined by the six constituent atoms. The dihedral angle formed by the benzofuran ring system and the 3-methylphenyl ring is 79.09 (5)°. In the crystal structure (Fig. 2), molecules are linked along the *c*-axis direction by two different inversion-generated pairs of C–H \cdots π hydrogen bonds (Table 1, Cg1 is the centroid of the C11–C16 3-methylphenyl ring), and π – π interactions between the benzene and furan rings of neighbouring molecules, with a Cg2 \cdots Cg3ⁱⁱ distance of 3.673 (2) Å and an interplanar distance of 3.570 (2) Å resulting in a slippage of 0.864 (2) Å (Cg2 and Cg3 are the centroids of the C2–C7 benzene ring and the C1/C2/C7/O1/C8 furan ring, respectively). In addition, intramolecular C–H \cdots O hydrogen bonds (Table 1) are observed.

S2. Experimental

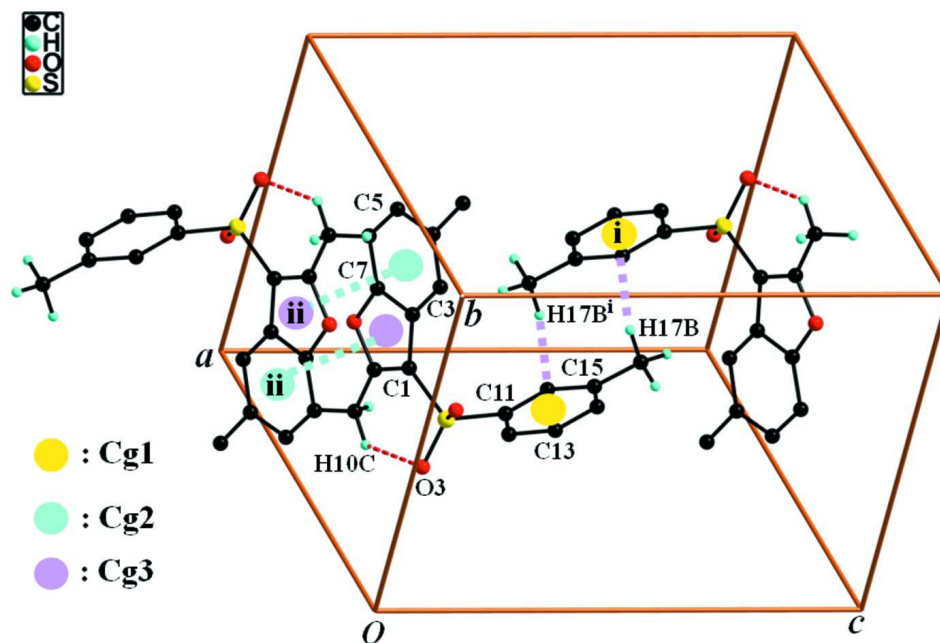
The starting material 2,5-dimethyl-3-(3-methylphenylsulfonyl)-1-benzofuran was prepared by literature method (Choi *et al.* 1999). 3-Chloroperoxybenzoic acid (77%, 515 mg, 2.3 mmol) was added in small portions to a stirred solution of 2,5-dimethyl-3-(3-methylphenylsulfonyl)-1-benzofuran (295 mg, 1.1 mmol) in dichloromethane (30 mL) at 273 K. After being stirred at room temperature for 8h, the mixture was washed with saturated sodium bicarbonate solution (2 X 20 mL) 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 73% (241 mg); m.p. 378–379 K; R_f = 0.43 (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 (28 mg) in acetone (15 mL) 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_{iso} (H) = 1.2 U_{eq} (C) for aryl and 1.5 U_{eq} (C) for methyl H atoms. The positions of methyl hydrogens were optimized using the SHELXL-97's command AFIX 137 (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 \cdots O, C–H \cdots 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) $-x + 1, -y + 1, -z + 1$; (ii) $-x + 1, -y + 1, -z$.]

2,5-Dimethyl-3-(3-methylphenylsulfonyl)-1-benzofuran

Crystal data

C₁₇H₁₆O₃S $M_r = 300.36$ Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

 $a = 9.8769$ (2) Å $b = 11.3190$ (2) Å $c = 13.1320$ (2) Å $\beta = 101.951$ (1)° $V = 1436.29$ (4) Å³ $Z = 4$ $F(000) = 632$ $D_x = 1.389$ Mg m⁻³

Melting point = 378–379 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3458 reflections

 $\theta = 2.4$ – 25.7 ° $\mu = 0.23$ mm⁻¹ $T = 173$ K

Block, colourless

 $0.33 \times 0.29 \times 0.23$ 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 scansAbsorption correction: multi-scan
(SADABS; Bruker, 2009) $T_{\min} = 0.927$, $T_{\max} = 0.947$

13810 measured reflections

3589 independent reflections

2861 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.035$ $\theta_{\max} = 28.4$ °, $\theta_{\min} = 2.4$ ° $h = -13 \rightarrow 12$ $k = -14 \rightarrow 15$ $l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.045$ $wR(F^2) = 0.128$ $S = 1.08$

3589 reflections

193 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

 $w = 1/[\sigma^2(F_o^2) + (0.0639P)^2 + 0.4013P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.35$ e Å⁻³ $\Delta\rho_{\min} = -0.39$ e Å⁻³

Special details

Experimental. ¹H NMR (δ p.p.m., CDCl₃, 400 Hz): 7.77–7.83 (m, 2H), 7.67 (s, 1H), 7.34–7.41 (m, 2H), 7.29 (d, $J = 8.56$ Hz, 1H), 7.10 (dd, $J = 8.56$ Hz and 1.72 Hz, 1H), 2.78 (s, 3H), 2.45 (s, 3H), 2.40 (s, 3H).**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	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.29608 (4)	0.36272 (4)	0.17488 (3)	0.02967 (14)
O1	0.66012 (13)	0.37182 (11)	0.09943 (10)	0.0345 (3)

O2	0.20801 (13)	0.46348 (11)	0.14867 (10)	0.0366 (3)
O3	0.24998 (14)	0.24951 (11)	0.13176 (10)	0.0384 (3)
C1	0.45457 (18)	0.39515 (16)	0.14324 (12)	0.0287 (4)
C2	0.52013 (17)	0.51022 (15)	0.14998 (12)	0.0273 (4)
C3	0.48710 (18)	0.62452 (15)	0.17608 (13)	0.0297 (4)
H3	0.4006	0.6408	0.1940	0.036*
C4	0.58250 (19)	0.71390 (16)	0.17537 (13)	0.0306 (4)
C5	0.70909 (19)	0.68878 (18)	0.14708 (14)	0.0356 (4)
H5	0.7734	0.7511	0.1468	0.043*
C6	0.74318 (19)	0.57618 (17)	0.11965 (14)	0.0361 (4)
H6	0.8287	0.5597	0.1003	0.043*
C7	0.64635 (19)	0.48979 (16)	0.12196 (13)	0.0306 (4)
C8	0.54295 (19)	0.31645 (16)	0.11373 (13)	0.0315 (4)
C9	0.5504 (2)	0.83842 (17)	0.20414 (15)	0.0385 (4)
H9A	0.4861	0.8749	0.1458	0.058*
H9B	0.6362	0.8845	0.2199	0.058*
H9C	0.5082	0.8367	0.2654	0.058*
C10	0.5398 (2)	0.18729 (17)	0.09586 (16)	0.0410 (5)
H10A	0.6052	0.1485	0.1523	0.062*
H10B	0.5660	0.1704	0.0293	0.062*
H10C	0.4463	0.1574	0.0941	0.062*
C11	0.33565 (18)	0.34750 (15)	0.31193 (14)	0.0293 (4)
C12	0.3862 (2)	0.24005 (16)	0.35446 (15)	0.0350 (4)
H12	0.3997	0.1762	0.3107	0.042*
C13	0.4166 (2)	0.22735 (18)	0.46169 (15)	0.0405 (5)
H13	0.4527	0.1549	0.4922	0.049*
C14	0.3941 (2)	0.32033 (18)	0.52383 (15)	0.0383 (4)
H14	0.4147	0.3104	0.5973	0.046*
C15	0.34268 (18)	0.42744 (16)	0.48270 (14)	0.0321 (4)
C16	0.31430 (18)	0.44131 (16)	0.37446 (14)	0.0306 (4)
H16	0.2806	0.5146	0.3441	0.037*
C17	0.3154 (2)	0.52658 (18)	0.55131 (15)	0.0387 (4)
H17A	0.2158	0.5323	0.5488	0.058*
H17B	0.3486	0.6009	0.5270	0.058*
H17C	0.3641	0.5114	0.6230	0.058*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0298 (2)	0.0263 (2)	0.0322 (2)	-0.00279 (17)	0.00464 (17)	-0.00376 (16)
O1	0.0356 (7)	0.0348 (7)	0.0345 (6)	0.0044 (5)	0.0105 (5)	-0.0018 (5)
O2	0.0326 (7)	0.0328 (7)	0.0437 (7)	0.0038 (5)	0.0062 (6)	0.0015 (6)
O3	0.0415 (8)	0.0308 (7)	0.0403 (7)	-0.0082 (6)	0.0027 (6)	-0.0085 (6)
C1	0.0305 (9)	0.0286 (9)	0.0259 (8)	-0.0005 (7)	0.0036 (7)	-0.0013 (6)
C2	0.0276 (8)	0.0302 (9)	0.0230 (7)	0.0000 (7)	0.0026 (6)	0.0015 (6)
C3	0.0278 (9)	0.0307 (9)	0.0301 (8)	-0.0001 (7)	0.0050 (7)	-0.0002 (7)
C4	0.0318 (9)	0.0306 (9)	0.0272 (8)	-0.0003 (7)	0.0008 (7)	0.0040 (7)
C5	0.0327 (9)	0.0371 (11)	0.0367 (9)	-0.0059 (8)	0.0066 (7)	0.0085 (8)

C6	0.0315 (9)	0.0431 (11)	0.0355 (9)	0.0018 (8)	0.0109 (7)	0.0062 (8)
C7	0.0340 (9)	0.0333 (10)	0.0247 (8)	0.0047 (8)	0.0064 (7)	0.0024 (7)
C8	0.0349 (9)	0.0317 (10)	0.0268 (8)	0.0014 (8)	0.0035 (7)	-0.0018 (7)
C9	0.0408 (11)	0.0325 (10)	0.0415 (10)	-0.0034 (8)	0.0066 (8)	0.0004 (8)
C10	0.0458 (11)	0.0337 (11)	0.0427 (10)	0.0065 (9)	0.0075 (9)	-0.0075 (8)
C11	0.0277 (9)	0.0279 (9)	0.0330 (8)	-0.0063 (7)	0.0078 (7)	-0.0021 (7)
C12	0.0384 (10)	0.0289 (10)	0.0391 (9)	-0.0042 (8)	0.0112 (8)	-0.0014 (8)
C13	0.0472 (12)	0.0335 (11)	0.0416 (10)	-0.0008 (9)	0.0115 (9)	0.0056 (8)
C14	0.0392 (10)	0.0424 (11)	0.0348 (9)	-0.0034 (9)	0.0110 (8)	0.0037 (8)
C15	0.0263 (8)	0.0358 (10)	0.0357 (9)	-0.0053 (7)	0.0098 (7)	-0.0051 (8)
C16	0.0282 (9)	0.0282 (9)	0.0359 (9)	-0.0032 (7)	0.0079 (7)	-0.0016 (7)
C17	0.0403 (11)	0.0411 (11)	0.0363 (9)	-0.0004 (9)	0.0115 (8)	-0.0036 (8)

Geometric parameters (Å, °)

S1—O2	1.4324 (13)	C9—H9B	0.9800
S1—O3	1.4364 (13)	C9—H9C	0.9800
S1—C1	1.7399 (18)	C10—H10A	0.9800
S1—C11	1.7693 (18)	C10—H10B	0.9800
O1—C8	1.363 (2)	C10—H10C	0.9800
O1—C7	1.380 (2)	C11—C16	1.385 (2)
C1—C8	1.359 (2)	C11—C12	1.387 (3)
C1—C2	1.449 (2)	C12—C13	1.385 (3)
C2—C7	1.390 (2)	C12—H12	0.9500
C2—C3	1.394 (2)	C13—C14	1.378 (3)
C3—C4	1.384 (2)	C13—H13	0.9500
C3—H3	0.9500	C14—C15	1.381 (3)
C4—C5	1.405 (3)	C14—H14	0.9500
C4—C9	1.510 (3)	C15—C16	1.399 (2)
C5—C6	1.385 (3)	C15—C17	1.498 (3)
C5—H5	0.9500	C16—H16	0.9500
C6—C7	1.372 (3)	C17—H17A	0.9800
C6—H6	0.9500	C17—H17B	0.9800
C8—C10	1.480 (3)	C17—H17C	0.9800
C9—H9A	0.9800		
O2—S1—O3	119.24 (8)	C4—C9—H9C	109.5
O2—S1—C1	107.84 (8)	H9A—C9—H9C	109.5
O3—S1—C1	108.75 (9)	H9B—C9—H9C	109.5
O2—S1—C11	108.50 (8)	C8—C10—H10A	109.5
O3—S1—C11	107.42 (8)	C8—C10—H10B	109.5
C1—S1—C11	104.08 (8)	H10A—C10—H10B	109.5
C8—O1—C7	106.93 (14)	C8—C10—H10C	109.5
C8—C1—C2	107.54 (16)	H10A—C10—H10C	109.5
C8—C1—S1	126.36 (15)	H10B—C10—H10C	109.5
C2—C1—S1	125.99 (13)	C16—C11—C12	121.31 (17)
C7—C2—C3	119.19 (17)	C16—C11—S1	119.99 (14)
C7—C2—C1	104.37 (15)	C12—C11—S1	118.70 (13)

C3—C2—C1	136.45 (16)	C13—C12—C11	118.97 (17)
C4—C3—C2	118.84 (17)	C13—C12—H12	120.5
C4—C3—H3	120.6	C11—C12—H12	120.5
C2—C3—H3	120.6	C14—C13—C12	119.69 (19)
C3—C4—C5	119.88 (17)	C14—C13—H13	120.2
C3—C4—C9	120.16 (17)	C12—C13—H13	120.2
C5—C4—C9	119.95 (17)	C13—C14—C15	122.04 (18)
C6—C5—C4	122.18 (17)	C13—C14—H14	119.0
C6—C5—H5	118.9	C15—C14—H14	119.0
C4—C5—H5	118.9	C14—C15—C16	118.42 (17)
C7—C6—C5	116.23 (17)	C14—C15—C17	121.33 (17)
C7—C6—H6	121.9	C16—C15—C17	120.24 (17)
C5—C6—H6	121.9	C11—C16—C15	119.54 (17)
C6—C7—O1	125.76 (17)	C11—C16—H16	120.2
C6—C7—C2	123.67 (18)	C15—C16—H16	120.2
O1—C7—C2	110.56 (16)	C15—C17—H17A	109.5
C1—C8—O1	110.60 (16)	C15—C17—H17B	109.5
C1—C8—C10	134.37 (18)	H17A—C17—H17B	109.5
O1—C8—C10	115.02 (16)	C15—C17—H17C	109.5
C4—C9—H9A	109.5	H17A—C17—H17C	109.5
C4—C9—H9B	109.5	H17B—C17—H17C	109.5
H9A—C9—H9B	109.5		
O2—S1—C1—C8	-150.31 (15)	C1—C2—C7—O1	-0.07 (18)
O3—S1—C1—C8	-19.69 (18)	C2—C1—C8—O1	-0.81 (19)
C11—S1—C1—C8	94.58 (16)	S1—C1—C8—O1	-177.28 (12)
O2—S1—C1—C2	33.86 (17)	C2—C1—C8—C10	178.18 (19)
O3—S1—C1—C2	164.48 (14)	S1—C1—C8—C10	1.7 (3)
C11—S1—C1—C2	-81.25 (16)	C7—O1—C8—C1	0.77 (18)
C8—C1—C2—C7	0.53 (18)	C7—O1—C8—C10	-178.44 (15)
S1—C1—C2—C7	177.01 (12)	O2—S1—C11—C16	-16.89 (17)
C8—C1—C2—C3	-179.26 (19)	O3—S1—C11—C16	-147.04 (14)
S1—C1—C2—C3	-2.8 (3)	C1—S1—C11—C16	97.75 (15)
C7—C2—C3—C4	-1.3 (2)	O2—S1—C11—C12	162.26 (14)
C1—C2—C3—C4	178.44 (18)	O3—S1—C11—C12	32.11 (17)
C2—C3—C4—C5	1.0 (3)	C1—S1—C11—C12	-83.10 (15)
C2—C3—C4—C9	-179.47 (15)	C16—C11—C12—C13	-0.5 (3)
C3—C4—C5—C6	-0.2 (3)	S1—C11—C12—C13	-179.62 (15)
C9—C4—C5—C6	-179.74 (17)	C11—C12—C13—C14	1.1 (3)
C4—C5—C6—C7	-0.2 (3)	C12—C13—C14—C15	-0.5 (3)
C5—C6—C7—O1	-178.79 (16)	C13—C14—C15—C16	-0.7 (3)
C5—C6—C7—C2	-0.1 (3)	C13—C14—C15—C17	178.39 (19)
C8—O1—C7—C6	178.39 (17)	C12—C11—C16—C15	-0.7 (3)
C8—O1—C7—C2	-0.41 (18)	S1—C11—C16—C15	178.42 (13)
C3—C2—C7—C6	0.9 (3)	C14—C15—C16—C11	1.3 (3)
C1—C2—C7—C6	-178.90 (16)	C17—C15—C16—C11	-177.82 (16)
C3—C2—C7—O1	179.76 (14)		

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C11–C16 3-methylphenyl ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C10—H10C···O3	0.98	2.34	3.078 (3)	131
C17—H17B···Cg1 ⁱ	0.98	2.88	3.478 (2)	121

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