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1-(4-Bromophenyl)-2-(phenylsulfonyl)-ethanone

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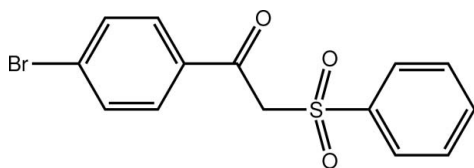
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.039; wR factor = 0.108; data-to-parameter ratio = 14.7.

The overall conformation of the title molecule, $\text{C}_{14}\text{H}_{11}\text{BrO}_3\text{S}$, is L-shaped, as seen in the value of the dihedral angle formed between the terminal benzene rings of 75.44 (13)°. The presence of $\text{C}-\text{H}\cdots\text{O}$ interactions leads to the formation of linear supramolecular chains along the a -axis direction in the crystal structure. These are connected into supramolecular arrays in the ab plane via $\text{C}-\text{H}\cdots\pi$ contacts.

Related literature

For the biological activity of sulphones, see: Garuti *et al.* (2002); Abdel-Aziz & Mekawey (2009); Abdel-Aziz *et al.* (2010). For the synthesis, see: Takahashi *et al.* (1986).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{11}\text{BrO}_3\text{S}$
 $M_r = 339.20$
Triclinic, $P\bar{1}$
 $a = 5.6467$ (4) Å
 $b = 10.3597$ (6) Å

$c = 11.1934$ (6) Å
 $\alpha = 86.430$ (5)°
 $\beta = 89.177$ (5)°
 $\gamma = 83.763$ (5)°
 $V = 649.64$ (7) Å³

$Z = 2$
Cu $K\alpha$ radiation
 $\mu = 5.83$ mm⁻¹

$T = 100$ K
 $0.25 \times 0.20 \times 0.02$ mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
 $T_{\min} = 0.291$, $T_{\max} = 1.000$

4181 measured reflections
2533 independent reflections
2396 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.108$
 $S = 1.04$
2533 reflections

172 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.69$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.80$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C9–C14 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C7}-\text{H7a}\cdots\text{O1}^{\text{i}}$	0.99	2.29	3.250 (3)	162
$\text{C7}-\text{H7b}\cdots\text{O1}^{\text{ii}}$	0.99	2.47	3.307 (3)	142
$\text{C4}-\text{H4}\cdots\text{Cg1}^{\text{iii}}$	0.95	2.87	3.708 (3)	147

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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, 2006); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2446).

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supporting information

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1-(4-Bromophenyl)-2-(phenylsulfonyl)ethanone

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S1. Comment

The analysis of the title compound, was prompted by the biological activity displayed by sulphones (Garuti, *et al.*, 2002; Abdel-Aziz & Mekawey, 2009; Abdel-Aziz *et al.*, 2010).

In the title molecule (Fig. 1), both sulfonyl-O atoms lie to one side of the S-bound benzene ring, and the methylene group to the other. The dihedral angle formed between the benzene rings of $75.44(13)^\circ$ is consistent with the molecule having an overall *L*-shape.

Supramolecular chains aligned along the *a* axis are the most predominant feature of the crystal packing (Table 1 and Fig. 2). Molecules are connected into a linear chain by an alternating sequence of centrosymmetric eight-membered $\{\cdots\text{HCH}\cdots\text{O}\}_2$ and $\{\cdots\text{HCSO}\}_2$ synthons. Chains are linked into layers in the *ab* plane by $\text{C}\cdots\text{H}\cdots\pi$ involving the S-bound and Br-benzene rings as donors and acceptors, respectively.

S2. Experimental

The title compound was prepared according to the reported method (Takahashi *et al.*, 1986). The crystals were isolated from its EtOH/DMF (*v/v* = 5/1) solution by slow evaporation at room temperature.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [$\text{C}\cdots\text{H}$ 0.95 to 0.99 Å, $U_{\text{iso}}(\text{H}) 1.2U_{\text{eq}}(\text{C})$] and were included in the refinement in the riding model approximation.

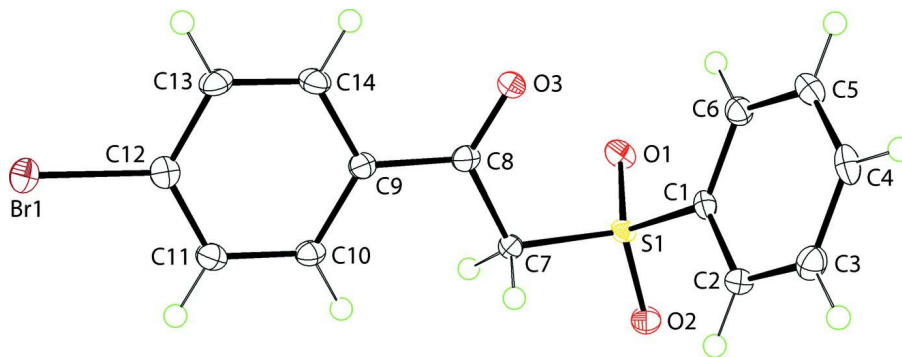


Figure 1

The molecular structure of the title compound showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

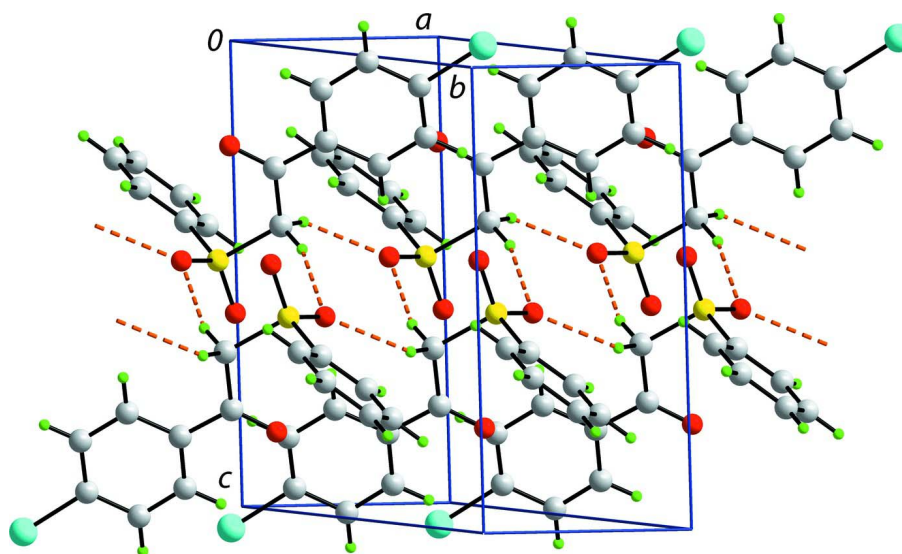


Figure 2

Supramolecular chain of the title molecules mediated by C—H \cdots O interactions, shown as orange lines.

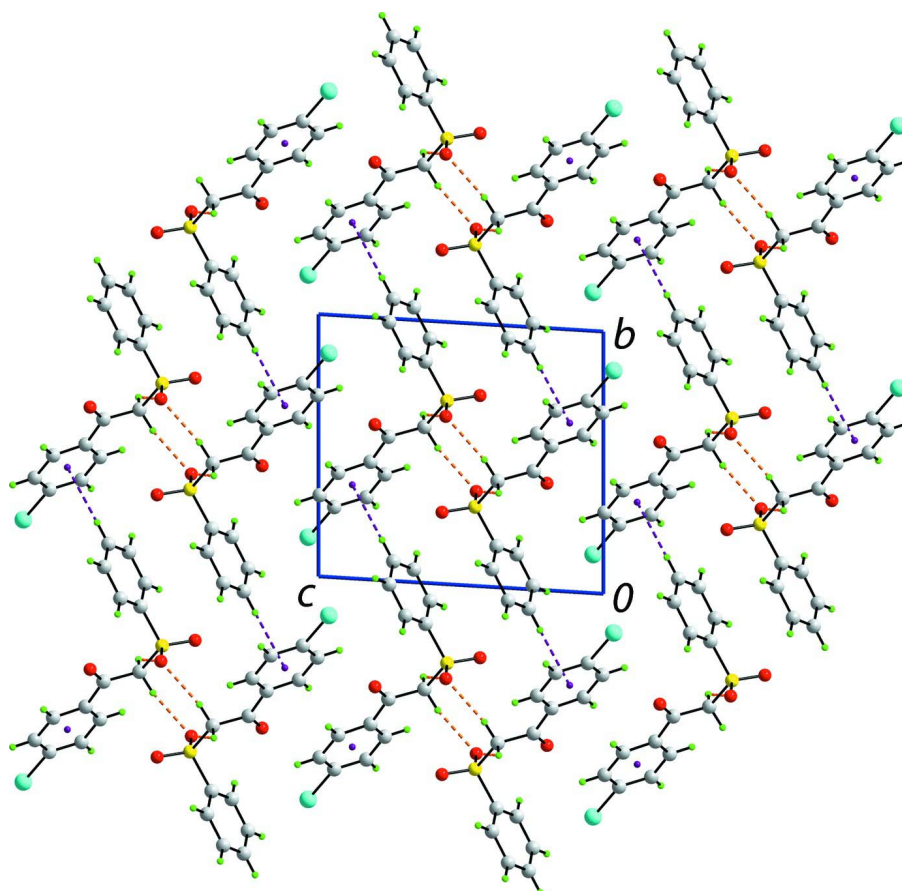


Figure 3

A view in projection down the a axis of the unit-cell contents of the title compound. The C—H \cdots O and C—H \cdots π interactions are shown as orange and purple dashed lines, respectively.

1-(4-Bromophenyl)-2-(phenylsulfonyl)ethanone

Crystal data

C₁₄H₁₁BrO₃S $M_r = 339.20$ Triclinic, $P\bar{1}$

Hall symbol: -P 1

 $a = 5.6467$ (4) Å $b = 10.3597$ (6) Å $c = 11.1934$ (6) Å $\alpha = 86.430$ (5)° $\beta = 89.177$ (5)° $\gamma = 83.763$ (5)° $V = 649.64$ (7) Å³ $Z = 2$ $F(000) = 340$ $D_x = 1.734$ Mg m⁻³Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å

Cell parameters from 2772 reflections

 $\theta = 4.0$ – 74.2 ° $\mu = 5.83$ mm⁻¹ $T = 100$ K

Plate, light-brown

 $0.25 \times 0.20 \times 0.02$ mm

Data collection

Agilent SuperNova Dual
diffractometer with Atlas detector
Radiation source: SuperNova (Cu) X-ray
Source

Mirror monochromator

Detector resolution: 10.4041 pixels mm⁻¹ ω scan

Absorption correction: multi-scan

(CrysAlis PRO; Agilent, 2010)

 $T_{\min} = 0.291$, $T_{\max} = 1.000$

4181 measured reflections

2533 independent reflections

2396 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.034$ $\theta_{\max} = 74.4$ °, $\theta_{\min} = 4.0$ ° $h = -7 \rightarrow 7$ $k = -12 \rightarrow 6$ $l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.039$ $wR(F^2) = 0.108$ $S = 1.04$

2533 reflections

172 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0821P)^2 + 0.0577P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.69$ e Å⁻³ $\Delta\rho_{\min} = -0.80$ e Å⁻³

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	1.22639 (4)	0.85297 (2)	-0.03616 (2)	0.01909 (14)
S1	0.56382 (10)	0.30122 (6)	0.45101 (5)	0.01267 (17)
O1	0.3196 (3)	0.36055 (18)	0.44650 (17)	0.0179 (4)

O2	0.6741 (3)	0.27303 (18)	0.56677 (16)	0.0187 (4)
O3	0.5107 (3)	0.40819 (18)	0.19816 (16)	0.0193 (4)
C1	0.5826 (4)	0.1561 (2)	0.3754 (2)	0.0137 (5)
C2	0.7865 (5)	0.0678 (3)	0.3911 (2)	0.0168 (5)
H2	0.9129	0.0869	0.4399	0.020*
C3	0.8018 (5)	-0.0480 (3)	0.3345 (2)	0.0198 (5)
H3	0.9389	-0.1094	0.3449	0.024*
C4	0.6160 (5)	-0.0744 (3)	0.2624 (3)	0.0195 (5)
H4	0.6276	-0.1534	0.2228	0.023*
C5	0.4139 (5)	0.0141 (3)	0.2480 (2)	0.0178 (5)
H5	0.2877	-0.0051	0.1991	0.021*
C6	0.3948 (4)	0.1304 (2)	0.3045 (2)	0.0164 (5)
H6	0.2567	0.1911	0.2950	0.020*
C7	0.7509 (5)	0.4054 (2)	0.3716 (2)	0.0137 (5)
H7A	0.7601	0.4828	0.4182	0.016*
H7B	0.9134	0.3591	0.3678	0.016*
C8	0.6743 (4)	0.4514 (2)	0.2452 (2)	0.0147 (5)
C9	0.8097 (4)	0.5513 (2)	0.1824 (2)	0.0143 (5)
C10	1.0105 (5)	0.5959 (3)	0.2326 (2)	0.0158 (5)
H10	1.0623	0.5639	0.3103	0.019*
C11	1.1329 (5)	0.6872 (3)	0.1681 (2)	0.0173 (5)
H11	1.2680	0.7183	0.2016	0.021*
C12	1.0565 (5)	0.7321 (2)	0.0551 (2)	0.0162 (5)
C13	0.8565 (5)	0.6902 (3)	0.0040 (2)	0.0184 (5)
H13	0.8051	0.7228	-0.0736	0.022*
C14	0.7355 (5)	0.6008 (3)	0.0685 (2)	0.0181 (5)
H14	0.5984	0.5720	0.0349	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0211 (2)	0.0184 (2)	0.01762 (19)	-0.00312 (12)	0.00239 (12)	0.00122 (12)
S1	0.0132 (3)	0.0128 (3)	0.0125 (3)	-0.0021 (2)	-0.0015 (2)	-0.0028 (2)
O1	0.0136 (9)	0.0173 (9)	0.0232 (9)	0.0003 (7)	0.0005 (7)	-0.0078 (7)
O2	0.0231 (10)	0.0203 (10)	0.0133 (9)	-0.0045 (7)	-0.0034 (7)	-0.0013 (7)
O3	0.0230 (9)	0.0170 (9)	0.0191 (9)	-0.0066 (7)	-0.0078 (7)	0.0003 (7)
C1	0.0163 (11)	0.0117 (11)	0.0139 (11)	-0.0044 (9)	0.0012 (9)	-0.0017 (8)
C2	0.0166 (12)	0.0173 (12)	0.0168 (12)	-0.0036 (10)	-0.0043 (9)	0.0008 (9)
C3	0.0198 (12)	0.0163 (13)	0.0226 (13)	0.0002 (10)	0.0012 (10)	0.0002 (10)
C4	0.0250 (14)	0.0144 (12)	0.0206 (12)	-0.0081 (10)	0.0056 (10)	-0.0046 (9)
C5	0.0178 (12)	0.0201 (13)	0.0171 (12)	-0.0075 (10)	0.0019 (9)	-0.0039 (9)
C6	0.0157 (12)	0.0164 (12)	0.0173 (12)	-0.0028 (9)	0.0001 (9)	-0.0009 (9)
C7	0.0151 (11)	0.0125 (11)	0.0138 (12)	-0.0026 (9)	-0.0024 (9)	-0.0011 (9)
C8	0.0169 (11)	0.0104 (11)	0.0164 (12)	0.0020 (9)	-0.0031 (9)	-0.0040 (9)
C9	0.0177 (12)	0.0108 (11)	0.0145 (12)	-0.0004 (9)	-0.0029 (9)	-0.0033 (9)
C10	0.0171 (12)	0.0169 (12)	0.0133 (11)	-0.0007 (9)	-0.0031 (9)	-0.0018 (9)
C11	0.0154 (12)	0.0182 (12)	0.0187 (13)	-0.0022 (9)	-0.0027 (9)	-0.0026 (10)
C12	0.0179 (12)	0.0145 (12)	0.0165 (12)	-0.0010 (9)	0.0019 (9)	-0.0039 (9)

C13	0.0228 (13)	0.0199 (13)	0.0125 (11)	-0.0011 (10)	-0.0052 (9)	-0.0012 (9)
C14	0.0183 (12)	0.0193 (12)	0.0175 (12)	-0.0035 (10)	-0.0058 (10)	-0.0031 (10)

Geometric parameters (Å, °)

Br1—C12	1.899 (3)	C6—H6	0.9500
S1—O2	1.4452 (19)	C7—C8	1.518 (3)
S1—O1	1.4478 (18)	C7—H7A	0.9900
S1—C1	1.763 (2)	C7—H7B	0.9900
S1—C7	1.781 (3)	C8—C9	1.489 (4)
O3—C8	1.210 (3)	C9—C14	1.397 (3)
C1—C6	1.392 (3)	C9—C10	1.407 (4)
C1—C2	1.396 (3)	C10—C11	1.391 (4)
C2—C3	1.386 (4)	C10—H10	0.9500
C2—H2	0.9500	C11—C12	1.379 (4)
C3—C4	1.393 (4)	C11—H11	0.9500
C3—H3	0.9500	C12—C13	1.395 (4)
C4—C5	1.389 (4)	C13—C14	1.372 (4)
C4—H4	0.9500	C13—H13	0.9500
C5—C6	1.388 (4)	C14—H14	0.9500
C5—H5	0.9500		
O2—S1—O1	118.37 (11)	S1—C7—H7A	108.3
O2—S1—C1	108.48 (11)	C8—C7—H7B	108.3
O1—S1—C1	108.42 (11)	S1—C7—H7B	108.3
O2—S1—C7	104.73 (11)	H7A—C7—H7B	107.4
O1—S1—C7	109.49 (12)	O3—C8—C9	121.8 (2)
C1—S1—C7	106.77 (11)	O3—C8—C7	121.2 (2)
C6—C1—C2	121.6 (2)	C9—C8—C7	117.0 (2)
C6—C1—S1	120.05 (19)	C14—C9—C10	119.0 (2)
C2—C1—S1	118.32 (18)	C14—C9—C8	118.4 (2)
C3—C2—C1	119.1 (2)	C10—C9—C8	122.6 (2)
C3—C2—H2	120.5	C11—C10—C9	119.8 (2)
C1—C2—H2	120.5	C11—C10—H10	120.1
C2—C3—C4	119.9 (2)	C9—C10—H10	120.1
C2—C3—H3	120.1	C12—C11—C10	119.4 (2)
C4—C3—H3	120.1	C12—C11—H11	120.3
C5—C4—C3	120.4 (2)	C10—C11—H11	120.3
C5—C4—H4	119.8	C11—C12—C13	121.8 (2)
C3—C4—H4	119.8	C11—C12—Br1	120.0 (2)
C4—C5—C6	120.5 (2)	C13—C12—Br1	118.2 (2)
C4—C5—H5	119.7	C14—C13—C12	118.5 (2)
C6—C5—H5	119.7	C14—C13—H13	120.7
C5—C6—C1	118.5 (2)	C12—C13—H13	120.7
C5—C6—H6	120.8	C13—C14—C9	121.4 (2)
C1—C6—H6	120.8	C13—C14—H14	119.3
C8—C7—S1	115.92 (18)	C9—C14—H14	119.3
C8—C7—H7A	108.3		

O2—S1—C1—C6	142.5 (2)	S1—C7—C8—O3	-7.5 (3)
O1—S1—C1—C6	12.8 (2)	S1—C7—C8—C9	172.60 (17)
C7—S1—C1—C6	-105.1 (2)	O3—C8—C9—C14	3.6 (3)
O2—S1—C1—C2	-36.0 (2)	C7—C8—C9—C14	-176.6 (2)
O1—S1—C1—C2	-165.7 (2)	O3—C8—C9—C10	-175.5 (3)
C7—S1—C1—C2	76.4 (2)	C7—C8—C9—C10	4.4 (3)
C6—C1—C2—C3	0.1 (4)	C14—C9—C10—C11	-0.6 (4)
S1—C1—C2—C3	178.6 (2)	C8—C9—C10—C11	178.4 (2)
C1—C2—C3—C4	0.5 (4)	C9—C10—C11—C12	-0.5 (4)
C2—C3—C4—C5	-0.8 (4)	C10—C11—C12—C13	1.1 (4)
C3—C4—C5—C6	0.5 (4)	C10—C11—C12—Br1	-178.25 (18)
C4—C5—C6—C1	0.1 (4)	C11—C12—C13—C14	-0.7 (4)
C2—C1—C6—C5	-0.4 (4)	Br1—C12—C13—C14	178.7 (2)
S1—C1—C6—C5	-178.86 (19)	C12—C13—C14—C9	-0.5 (4)
O2—S1—C7—C8	-179.65 (18)	C10—C9—C14—C13	1.1 (4)
O1—S1—C7—C8	-51.8 (2)	C8—C9—C14—C13	-178.0 (2)
C1—S1—C7—C8	65.4 (2)		

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C9–C14 ring.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C7—H7a \cdots O1 ⁱ	0.99	2.29	3.250 (3)	162
C7—H7b \cdots O1 ⁱⁱ	0.99	2.47	3.307 (3)	142
C4—H4 \cdots Cg1 ⁱⁱⁱ	0.95	2.87	3.708 (3)	147

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