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

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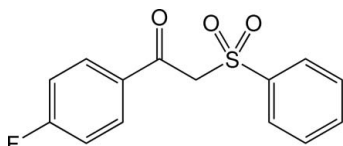
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.037; wR factor = 0.105; data-to-parameter ratio = 13.8.

In the title compound, $\text{C}_{14}\text{H}_{11}\text{FO}_3\text{S}$, the unit comprising the ethanone and 4-fluorophenyl groups is essentially planar, with an r.m.s. deviation of 0.0084 (2) Å for the ten non-H atoms, and it makes a dihedral angle of 37.31 (10)° with the phenyl ring. In the crystal, molecules are linked by pairs of weak C—H \cdots O hydrogen bonds into inversion dimers with $R_2^2(16)$ graph-set motifs. The dimers are stacked along the b axis through further C—H \cdots O hydrogen bonds.

Related literature

For bond-length data, see: Allen *et al.* (1987). For background to the chemistry of arylsulphones, see: Abdel-Aziz *et al.* (2009, 2010); Grandison *et al.* (2002); Silvestri *et al.* (2000); Stephens *et al.* (2001); Xiang *et al.* (2007). For related structures, see: Abdel-Aziz *et al.* (2011, 2012). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{11}\text{FO}_3\text{S}$ $c = 20.4401$ (5) Å
 $M_r = 278.30$ $\beta = 119.612$ (2)°
 Monoclinic, $P2_1/c$ $V = 1296.01$ (6) Å³
 $a = 13.7046$ (3) Å $Z = 4$
 $b = 5.3216$ (1) Å Cu $K\alpha$ radiation

$\mu = 2.36$ mm⁻¹
 $T = 296$ K

0.58 × 0.23 × 0.07 mm

Data collection

Bruker SMART APEXII CCD 8880 measured reflections
 area-detector diffractometer 2393 independent reflections
 Absorption correction: multi-scan 2090 reflections with $I > 2\sigma(I)$
 (SADABS; Bruker, 2009) $R_{\text{int}} = 0.033$
 $T_{\text{min}} = 0.341$, $T_{\text{max}} = 0.852$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$ 173 parameters
 $wR(F^2) = 0.105$ H-atom parameters constrained
 $S = 1.07$ $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 2393 reflections $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| D—H \cdots A | D—H | H \cdots A | D \cdots A | D—H \cdots A |
|----------------------------------|------|--------------|--------------|----------------|
| C1—H1B \cdots O3 ⁱ | 0.97 | 2.23 | 3.183 (2) | 168 |
| C5—H5A \cdots O2 ⁱⁱ | 0.93 | 2.57 | 3.218 (3) | 127 |

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5133).

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[§] Thomson Reuters ResearcherID: A-3561-2009.

supporting information

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

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S1. Comment

Arylsulphones are an interesting class of non-nucleoside antiviral agents. A large number of them have been also shown various interesting biological activities (Abdel-Aziz *et al.*, 2009, 2010; Silvestri *et al.*, 2000; Stephens *et al.*, 2001) and found application in membrane technology for nanofiltration (Grandison *et al.*, 2002). During the course of our research on the medicinal chemistry of arylsulphones, the title compound(I) was synthesized and studied for its biological activity. Herein the crystal structure of (I) was reported.

The title molecule has a fold structure as indicated by the dihedral angle between the 4-fluorophenyl and phenyl rings being $36.98(12)^\circ$ (Fig. 1). The ethanone unit [C1/C2/O1] lies on the same plane with the 4-fluorophenyl ring with an *r.m.s.* deviation of $0.0084(2)$ Å for the ten non-H atoms (C1–C8/O1/F1) and the dihedral angle between the ethanone plane and the 4-fluorophenyl ring being $1.2(2)^\circ$. The environment of S atom is a distorted tetrahedral geometry [angles around S atom are $105.67(8)$ – $118.24(9)^\circ$] being surrounded by two O atoms, one C atom of the ethanone unit and one C atom of the benzene ring. The bond distances in (I) are within normal ranges (Allen *et al.*, 1987) and comparable to the related structures (Abdel-Aziz *et al.*, 2011, 2012).

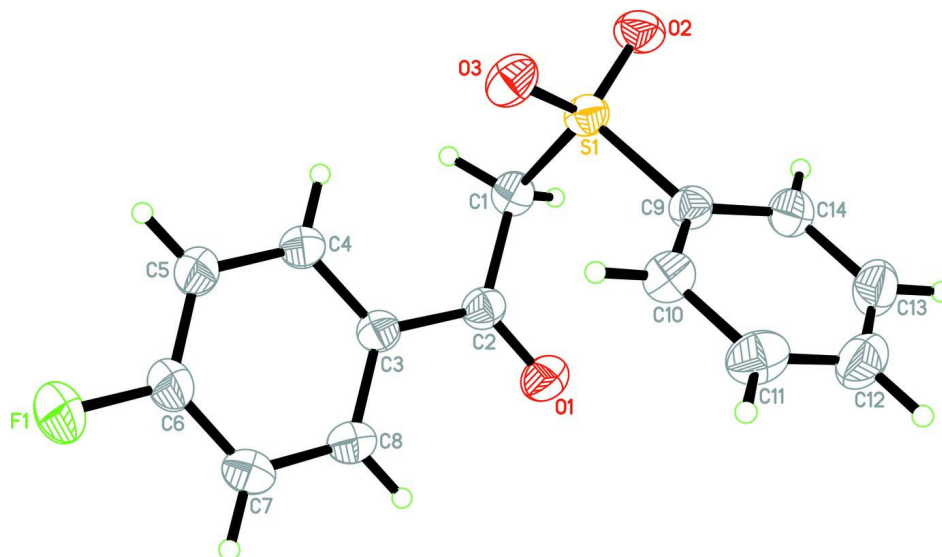
In the crystal packing (Fig. 2), the molecules are linked by pairs of weak $C\cdots H\cdots O_{\text{sulfonyl}}$ interactions (Table 1) into inversion dimers with $R_2^2(16)$ graph-set motifs (Bernstein *et al.*, 1995) and these dimers are arranged into layers parallel to the *ac* plane and stacked along the *b* axis.

S2. Experimental

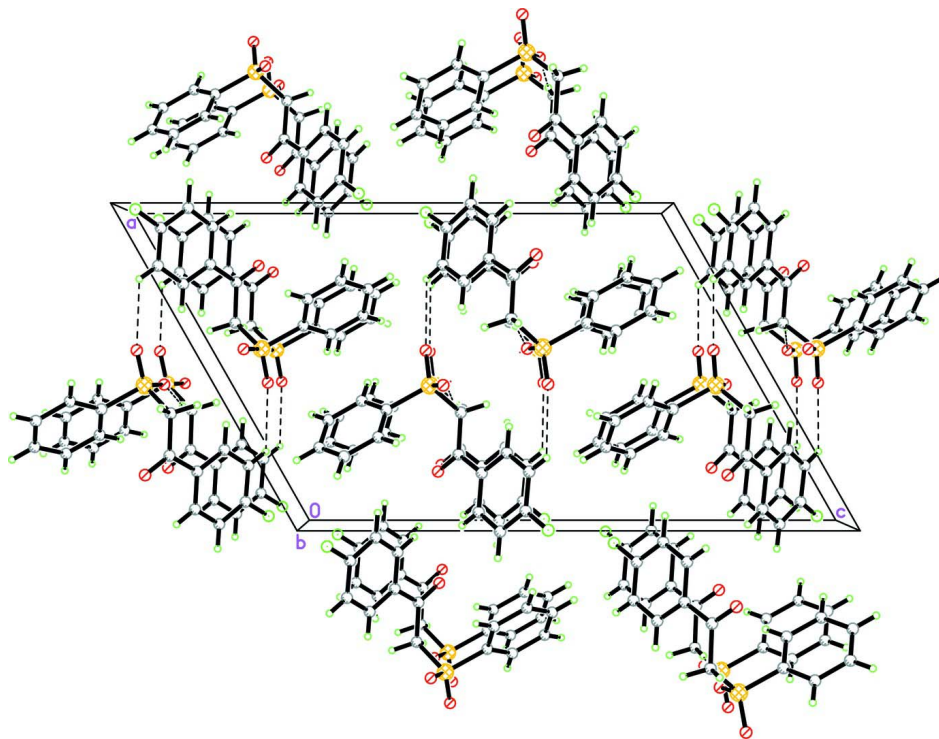
The title compound was prepared according to the reported method (Xiang *et al.*, 2007). Colorless plate-shaped single crystals suitable for an *X*-ray structural analysis were obtained by slow evaporation from an ethanol solution at room temperature.

S3. Refinement

H atoms were placed in calculated positions with $d(C-H) = 0.93$ for aromatic and 0.97 Å for CH_2 atoms. The $U_{\text{iso}}(H)$ values were constrained to be $1.2U_{\text{eq}}$ of the carrier atom.

**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

**Figure 2**

A crystal packing diagram of the title compound viewed along the *b* axis, showing molecular layers parallel to the *ac* plane. The C—H...O hydrogen bonds are shown by dashed lines.

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

Crystal data

C₁₄H₁₁FO₃S $M_r = 278.30$ Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

 $a = 13.7046$ (3) Å $b = 5.3216$ (1) Å $c = 20.4401$ (5) Å $\beta = 119.612$ (2)° $V = 1296.01$ (6) Å³ $Z = 4$ $F(000) = 576$ $D_x = 1.426$ Mg m⁻³Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 2393 reflections

 $\theta = 3.7$ – 71.2 ° $\mu = 2.36$ mm⁻¹ $T = 296$ K

Plate, colorless

 $0.58 \times 0.23 \times 0.07$ mm

Data collection

Bruker SMART APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scansAbsorption correction: multi-scan
(*SADABS*; Bruker, 2009) $T_{\min} = 0.341$, $T_{\max} = 0.852$

8880 measured reflections

2393 independent reflections

2090 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.033$ $\theta_{\text{max}} = 71.2$ °, $\theta_{\text{min}} = 3.7$ ° $h = -16 \rightarrow 16$ $k = -5 \rightarrow 6$ $l = -24 \rightarrow 25$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.037$ $wR(F^2) = 0.105$ $S = 1.07$

2393 reflections

173 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.2892P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³Extinction correction: *SHELXTL* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0041 (5)

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|--------------|-------------|--------------|----------------------------------|
| S1 | 0.55567 (3) | 0.70852 (8) | 0.61500 (2) | 0.04632 (18) |
| F1 | 0.96706 (13) | 0.1120 (4) | 0.55007 (10) | 0.1107 (6) |
| O1 | 0.81880 (12) | 0.9811 (3) | 0.68962 (8) | 0.0662 (4) |

| | | | | |
|------|--------------|------------|--------------|------------|
| O2 | 0.45075 (10) | 0.8367 (3) | 0.58825 (8) | 0.0616 (4) |
| O3 | 0.55394 (12) | 0.4560 (2) | 0.58997 (8) | 0.0603 (4) |
| C1 | 0.63784 (15) | 0.8990 (3) | 0.58896 (10) | 0.0492 (4) |
| H1A | 0.6133 | 0.8700 | 0.5362 | 0.059* |
| H1B | 0.6236 | 1.0741 | 0.5944 | 0.059* |
| C2 | 0.76418 (15) | 0.8516 (4) | 0.63472 (9) | 0.0492 (4) |
| C3 | 0.81547 (14) | 0.6528 (4) | 0.61084 (9) | 0.0488 (4) |
| C4 | 0.75317 (15) | 0.5065 (4) | 0.54707 (10) | 0.0540 (4) |
| H4A | 0.6762 | 0.5324 | 0.5178 | 0.065* |
| C5 | 0.80438 (17) | 0.3233 (4) | 0.52674 (11) | 0.0630 (5) |
| H5A | 0.7629 | 0.2242 | 0.4844 | 0.076* |
| C6 | 0.91764 (19) | 0.2912 (5) | 0.57045 (13) | 0.0716 (6) |
| C7 | 0.98184 (18) | 0.4289 (6) | 0.63456 (13) | 0.0798 (7) |
| H7A | 1.0585 | 0.3991 | 0.6638 | 0.096* |
| C8 | 0.93098 (16) | 0.6100 (5) | 0.65444 (12) | 0.0660 (6) |
| H8A | 0.9735 | 0.7059 | 0.6974 | 0.079* |
| C9 | 0.62748 (14) | 0.7076 (3) | 0.71439 (10) | 0.0470 (4) |
| C10 | 0.70719 (16) | 0.5235 (4) | 0.75248 (11) | 0.0560 (4) |
| H10A | 0.7222 | 0.4007 | 0.7263 | 0.067* |
| C11 | 0.76409 (19) | 0.5262 (5) | 0.83057 (12) | 0.0691 (6) |
| H11A | 0.8182 | 0.4049 | 0.8573 | 0.083* |
| C12 | 0.7406 (2) | 0.7079 (5) | 0.86849 (12) | 0.0718 (6) |
| H12A | 0.7791 | 0.7089 | 0.9208 | 0.086* |
| C13 | 0.6606 (2) | 0.8885 (5) | 0.82995 (13) | 0.0733 (6) |
| H13A | 0.6452 | 1.0099 | 0.8563 | 0.088* |
| C14 | 0.60266 (17) | 0.8904 (4) | 0.75166 (12) | 0.0596 (5) |
| H14A | 0.5485 | 1.0119 | 0.7252 | 0.072* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|---------------|
| S1 | 0.0442 (3) | 0.0421 (3) | 0.0460 (3) | 0.00262 (16) | 0.01715 (19) | -0.00338 (15) |
| F1 | 0.0781 (9) | 0.1412 (15) | 0.1014 (11) | 0.0380 (9) | 0.0356 (8) | -0.0343 (10) |
| O1 | 0.0622 (8) | 0.0691 (10) | 0.0584 (8) | -0.0055 (7) | 0.0229 (7) | -0.0153 (7) |
| O2 | 0.0431 (6) | 0.0673 (9) | 0.0636 (8) | 0.0067 (6) | 0.0181 (6) | -0.0023 (6) |
| O3 | 0.0713 (8) | 0.0437 (8) | 0.0575 (8) | -0.0013 (6) | 0.0253 (6) | -0.0084 (6) |
| C1 | 0.0533 (9) | 0.0428 (10) | 0.0480 (9) | 0.0091 (7) | 0.0222 (7) | 0.0055 (7) |
| C2 | 0.0498 (9) | 0.0508 (11) | 0.0437 (9) | -0.0009 (8) | 0.0207 (7) | 0.0027 (7) |
| C3 | 0.0446 (8) | 0.0566 (11) | 0.0415 (8) | 0.0032 (7) | 0.0184 (7) | 0.0025 (7) |
| C4 | 0.0449 (8) | 0.0656 (12) | 0.0445 (9) | 0.0057 (8) | 0.0168 (7) | -0.0008 (8) |
| C5 | 0.0577 (11) | 0.0790 (15) | 0.0482 (10) | 0.0086 (10) | 0.0229 (8) | -0.0076 (9) |
| C6 | 0.0606 (11) | 0.0879 (17) | 0.0655 (13) | 0.0192 (11) | 0.0305 (10) | -0.0078 (11) |
| C7 | 0.0468 (10) | 0.109 (2) | 0.0684 (13) | 0.0185 (11) | 0.0168 (9) | -0.0101 (13) |
| C8 | 0.0478 (10) | 0.0837 (16) | 0.0527 (10) | 0.0038 (10) | 0.0144 (8) | -0.0103 (10) |
| C9 | 0.0468 (8) | 0.0465 (10) | 0.0464 (9) | -0.0037 (7) | 0.0221 (7) | -0.0027 (7) |
| C10 | 0.0611 (10) | 0.0485 (11) | 0.0540 (10) | 0.0013 (8) | 0.0248 (8) | 0.0029 (8) |
| C11 | 0.0695 (12) | 0.0637 (14) | 0.0588 (12) | -0.0041 (10) | 0.0200 (10) | 0.0138 (10) |
| C12 | 0.0808 (15) | 0.0851 (17) | 0.0468 (10) | -0.0192 (12) | 0.0294 (10) | -0.0010 (10) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C13 | 0.0826 (15) | 0.0838 (17) | 0.0647 (13) | -0.0155 (13) | 0.0449 (12) | -0.0212 (12) |
| C14 | 0.0591 (10) | 0.0609 (13) | 0.0611 (11) | -0.0017 (9) | 0.0314 (9) | -0.0102 (9) |

Geometric parameters (Å, °)

| | | | |
|------------|-------------|--------------|-------------|
| S1—O2 | 1.4333 (13) | C6—C7 | 1.374 (3) |
| S1—O3 | 1.4342 (14) | C7—C8 | 1.364 (3) |
| S1—C9 | 1.7664 (17) | C7—H7A | 0.9300 |
| S1—C1 | 1.7807 (19) | C8—H8A | 0.9300 |
| F1—C6 | 1.349 (3) | C9—C14 | 1.378 (3) |
| O1—C2 | 1.210 (2) | C9—C10 | 1.385 (3) |
| C1—C2 | 1.528 (2) | C10—C11 | 1.388 (3) |
| C1—H1A | 0.9700 | C10—H10A | 0.9300 |
| C1—H1B | 0.9700 | C11—C12 | 1.374 (4) |
| C2—C3 | 1.480 (3) | C11—H11A | 0.9300 |
| C3—C4 | 1.391 (3) | C12—C13 | 1.376 (4) |
| C3—C8 | 1.399 (3) | C12—H12A | 0.9300 |
| C4—C5 | 1.380 (3) | C13—C14 | 1.391 (3) |
| C4—H4A | 0.9300 | C13—H13A | 0.9300 |
| C5—C6 | 1.366 (3) | C14—H14A | 0.9300 |
| C5—H5A | 0.9300 | | |
| O2—S1—O3 | 118.24 (9) | C5—C6—C7 | 122.8 (2) |
| O2—S1—C9 | 108.90 (9) | C8—C7—C6 | 118.70 (19) |
| O3—S1—C9 | 108.02 (8) | C8—C7—H7A | 120.7 |
| O2—S1—C1 | 106.18 (9) | C6—C7—H7A | 120.7 |
| O3—S1—C1 | 109.15 (9) | C7—C8—C3 | 120.62 (19) |
| C9—S1—C1 | 105.67 (8) | C7—C8—H8A | 119.7 |
| C2—C1—S1 | 114.57 (12) | C3—C8—H8A | 119.7 |
| C2—C1—H1A | 108.6 | C14—C9—C10 | 122.02 (18) |
| S1—C1—H1A | 108.6 | C14—C9—S1 | 118.98 (15) |
| C2—C1—H1B | 108.6 | C10—C9—S1 | 119.00 (14) |
| S1—C1—H1B | 108.6 | C9—C10—C11 | 118.5 (2) |
| H1A—C1—H1B | 107.6 | C9—C10—H10A | 120.7 |
| O1—C2—C3 | 122.41 (16) | C11—C10—H10A | 120.7 |
| O1—C2—C1 | 117.92 (17) | C12—C11—C10 | 120.1 (2) |
| C3—C2—C1 | 119.67 (15) | C12—C11—H11A | 120.0 |
| C4—C3—C8 | 118.88 (18) | C10—C11—H11A | 120.0 |
| C4—C3—C2 | 122.52 (16) | C11—C12—C13 | 120.8 (2) |
| C8—C3—C2 | 118.59 (17) | C11—C12—H12A | 119.6 |
| C5—C4—C3 | 120.65 (17) | C13—C12—H12A | 119.6 |
| C5—C4—H4A | 119.7 | C12—C13—C14 | 120.3 (2) |
| C3—C4—H4A | 119.7 | C12—C13—H13A | 119.9 |
| C6—C5—C4 | 118.29 (19) | C14—C13—H13A | 119.9 |
| C6—C5—H5A | 120.9 | C9—C14—C13 | 118.3 (2) |
| C4—C5—H5A | 120.9 | C9—C14—H14A | 120.8 |
| F1—C6—C5 | 117.9 (2) | C13—C14—H14A | 120.8 |
| F1—C6—C7 | 119.2 (2) | | |

| | | | |
|-------------|--------------|-----------------|--------------|
| O2—S1—C1—C2 | 159.03 (13) | C4—C3—C8—C7 | 0.4 (3) |
| O3—S1—C1—C2 | -72.49 (15) | C2—C3—C8—C7 | -180.0 (2) |
| C9—S1—C1—C2 | 43.46 (15) | O2—S1—C9—C14 | -23.82 (18) |
| S1—C1—C2—O1 | -93.21 (19) | O3—S1—C9—C14 | -153.41 (16) |
| S1—C1—C2—C3 | 87.07 (18) | C1—S1—C9—C14 | 89.87 (16) |
| O1—C2—C3—C4 | -178.92 (19) | O2—S1—C9—C10 | 156.30 (15) |
| C1—C2—C3—C4 | 0.8 (3) | O3—S1—C9—C10 | 26.71 (18) |
| O1—C2—C3—C8 | 1.5 (3) | C1—S1—C9—C10 | -90.01 (16) |
| C1—C2—C3—C8 | -178.84 (18) | C14—C9—C10—C11 | -0.6 (3) |
| C8—C3—C4—C5 | -0.5 (3) | S1—C9—C10—C11 | 179.24 (15) |
| C2—C3—C4—C5 | 179.91 (18) | C9—C10—C11—C12 | 0.3 (3) |
| C3—C4—C5—C6 | -0.5 (3) | C10—C11—C12—C13 | 0.2 (4) |
| C4—C5—C6—F1 | -179.9 (2) | C11—C12—C13—C14 | -0.4 (4) |
| C4—C5—C6—C7 | 1.7 (4) | C10—C9—C14—C13 | 0.4 (3) |
| F1—C6—C7—C8 | 179.8 (3) | S1—C9—C14—C13 | -179.46 (16) |
| C5—C6—C7—C8 | -1.8 (4) | C12—C13—C14—C9 | 0.1 (3) |
| C6—C7—C8—C3 | 0.7 (4) | | |

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|-------|-------------|-------------|---------------|
| C1—H1B \cdots O3 ⁱ | 0.97 | 2.23 | 3.183 (2) | 168 |
| C5—H5A \cdots O2 ⁱⁱ | 0.93 | 2.57 | 3.218 (3) | 127 |

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