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

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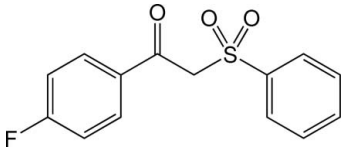
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.105; data-to-parameter ratio = 13.8.

In the title compound, $C_{14}H_{11}FO_3S$, 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···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···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

$C_{14}H_{11}FO_3S$
M_r = 278.30
Monoclinic, $P2_1/c$
a = 13.7046 (3) Å
b = 5.3216 (1) Å
c = 20.4401 (5) Å
β = 119.612 (2)°
V = 1296.01 (6) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.36 mm^{-1}
T = 296 K
0.58 × 0.23 × 0.07 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption 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_{int} = 0.033

Refinement

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···O3^{i}	0.97	2.23	3.183 (2)	168
C5—H5A···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.

supplementary materials

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

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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)° (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)°. The environment of S atom is a distorted tetrahedral geometry [angles around S atom are 105.67 (8)–118.24 (9)°] 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···H···$O_{sulfonyl}$ 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.

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.

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_{iso}(H) values were constrained to be $1.2U_{eq}$ of the carrier atom.

Computing details

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

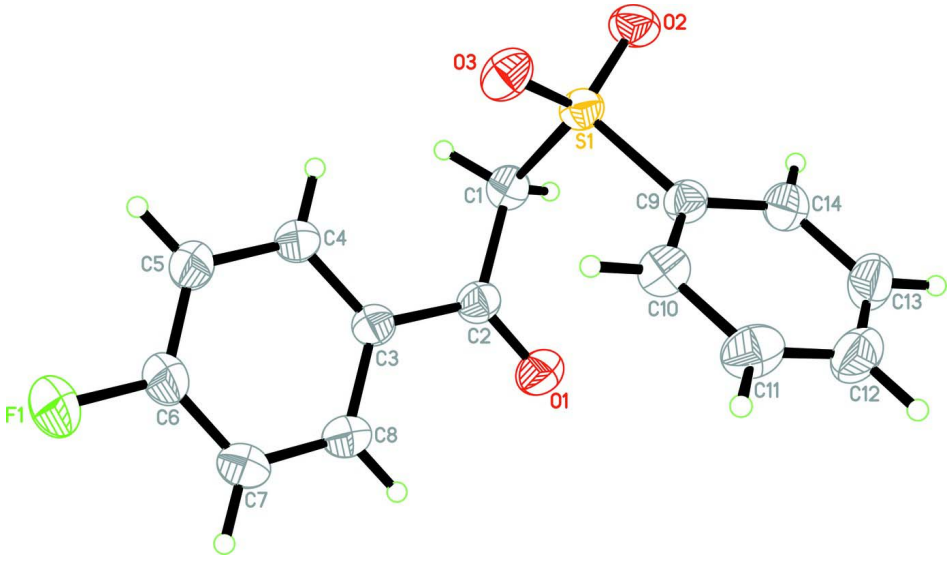

Figure 1

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

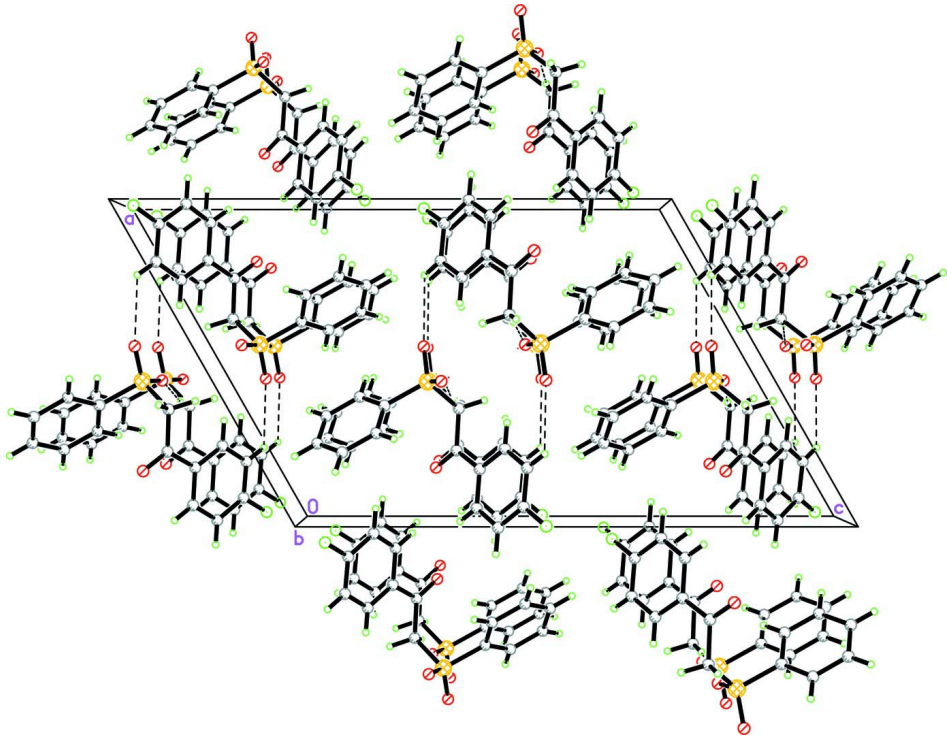

Figure 2

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

$C_{14}H_{11}FO_3S$
$M_r = 278.30$
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) Å^3
$Z = 4$
$F(000) = 576$
$D_x = 1.426$ Mg m^{-3}
Cu $K\alpha$ 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 × 0.23 × 0.07 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.341$, $T_{max} = 0.852$
8880 measured reflections
2393 independent reflections
2090 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 71.2°$, $\theta_{min} = 3.7°$
$h = -16 \rightarrow 16$
$k = -5 \rightarrow 6$
$l = -24 \rightarrow 25$

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 methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.2892P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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, º)

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 (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···O3^{i}	0.97	2.23	3.183 (2)	168
C5—H5*A*···O2^{ii}	0.93	2.57	3.218 (3)	127

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