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# 3-(4-Fluorophenylsulfonyl)-5-isopropyl-2-methyl-1-benzofuran

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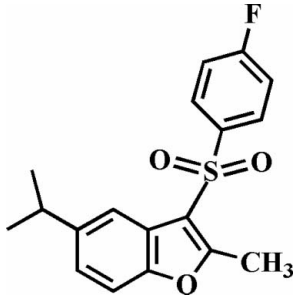
Key indicators: single-crystal X-ray study; $T$ = 175 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.037; $wR$ factor = 0.108; data-to-parameter ratio = 17.2.

In the title compound, $C_{18}H_{17}FO_3S$, the 4-fluorophenyl ring makes a dihedral angle of 82.12 (4)° with the plane of the benzofuran fragment. In the crystal structure, molecules are linked by weak intermolecular C—H···O hydrogen bonds and C—H···$\pi$ interactions.

## Related literature

For the crystal structures of similar 2-methyl-3-phenylsulfonyl-1-benzofuran derivatives, see: Choi *et al.* (2008*a*,*b*). For the biological activity of benzofuran compounds, see: Aslam *et al.* (2006); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003).




## Experimental

### Crystal data

$C_{18}H_{17}FO_3S$
$M_r$ = 332.38
Monoclinic, $P2_1/c$
$a$ = 10.9434 (6) Å
$b$ = 11.3395 (6) Å
$c$ = 13.0988 (7) Å
$\beta$ = 100.252 (3)°
$V$ = 1599.51 (15) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.23 mm$^{-1}$
$T$ = 175 K
0.41 × 0.29 × 0.17 mm

### Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.669, $T_{max}$ = 0.746
14304 measured reflections
3655 independent reflections
3109 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.030

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.108
$S$ = 1.02
3655 reflections
212 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

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

*Cg*1 and *Cg*2 are the centroids of the C1/C2/C7/O3/C8 furan ring and the C2–C7 benzene ring, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C14—H14···O2$^{i}$ | 0.95 | 2.51 | 3.401 (2) | 155 |
| C10—H10$B$···$Cg1^{ii}$ | 0.98 | 2.86 | 3.561 (2) | 120 |
| C11—H11$B$···$Cg2^{ii}$ | 0.98 | 2.91 | 3.670 (2) | 135 |
| C17—H17···$Cg2^{iii}$ | 0.95 | 2.89 | 3.528 (2) | 147 |

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

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: XU2750).

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# supporting information

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## 3-(4-Fluorophenylsulfonyl)-5-isopropyl-2-methyl-1-benzofuran

**Hong Dae Choi, Pil Ja Seo, Byeng Wha Son and Uk Lee**

### S1. Comment

The compounds containing benzofuran ring show potent biological activities such as antifungal (Aslam *et al.*, 2006), antitumor and antiviral (Galal *et al.*, 2009), antimicrobial (Khan *et al.*, 2005) properties. These compounds occur widely in nature (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing studies of the effect of side chain substituents on the solid state structures of 2-methyl-3-phenylsulfonyl-1-benzofuran analogues (Choi *et al.*, 2008*a*,*b*), we report the crystal structure of the title compound (Fig. 1).

The benzofuran unit is essentially planar, with a mean deviation of 0.113 (1) Å from the least-squares plane defined by the nine constituent atoms. The 4-fluorophenyl ring makes a dihedral angle of 82.12 (4)° with the plane of the benzofuran fragment. The molecular packing (Fig. 2) is stabilized by an intermolecular C—H···O hydrogen bond between the 4-fluorophenyl H atom and the oxygen of the sulfonyl group, with a C14—H14···O2$^{i}$ (Table 1). The crystal packing (Fig. 3) is further stabilized by three intermolecular C—H···$\pi$ interactions; the first one between the methyl H atom of the isopropyl group and the furan ring of an adjacent molecule, with a C10—H10B···Cg1$^{ii}$, the second one between the methyl H atom of the isopropyl group and the benzene ring of a neighbouring molecule, with a C11—H11B···Cg2$^{ii}$, and the third one between the 4-fluorophenyl H atom and the benzene ring of an adjacent benzofuran system, with a C17—H17···Cg2$^{iii}$, respectively (Table 1; Cg1 and Cg2 are the centroids of the C1/C2/C7/O3/C8 furan ring and the C2–C7 benzene ring, respectively).

### S2. Experimental

77% 3-Chloroperoxybenzoic acid (448 mg, 2.0 mmol) was added in small portions to a stirred solution of 3-(4-fluorophenylsulfanyl)-5-isoproyl-2-methyl-1-benzofuran (270 mg, 0.9 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 8 h, 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 (silica gel, hexane–ethyl acetate, 2:1 v/v) to afford the title compound as a colorless solid [yield 79%, m.p. 402–403 K; Rf = 0.69 (hexane–ethyl acetate, 2:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in benzene 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, 1.00 Å for methine and 0.98 Å for methyl H atoms, respectively. $U_{iso}$(H) = 1.2$U_{eq}$(C) for aryl and methine, and 1.5$U_{eq}$(C) for methyl H atoms.

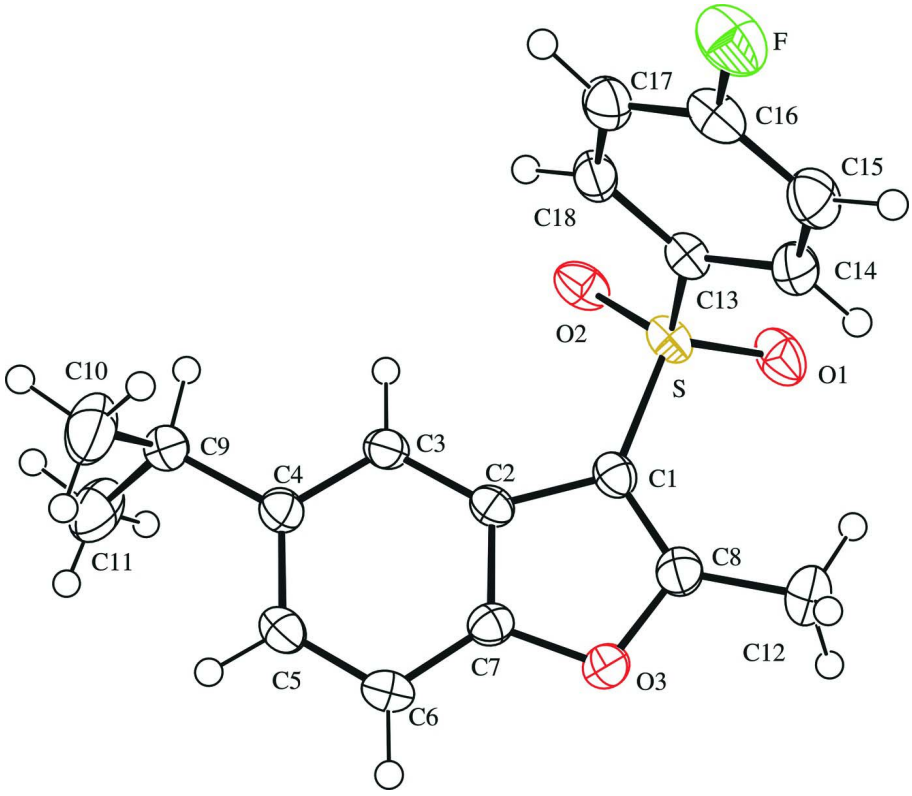


**Figure 1**

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 a small spheres of arbitrary radius.

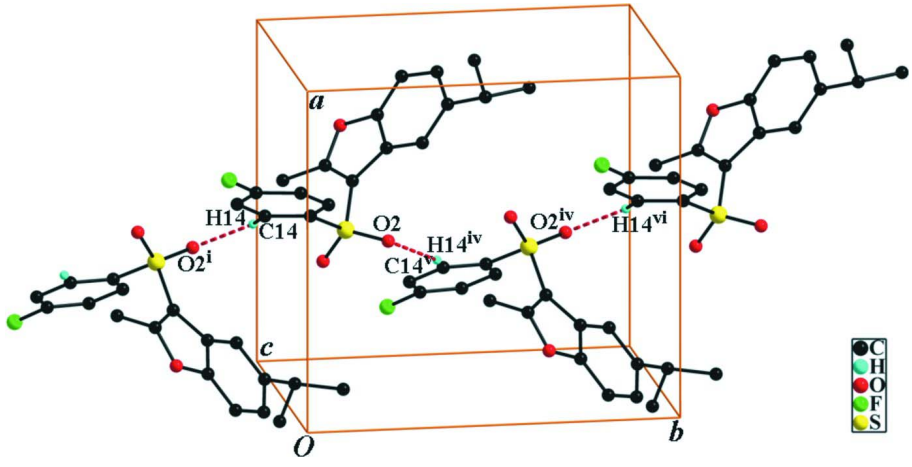


**Figure 2**

C—H···O interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) -*x* + 1, *y* - 1/2, -*z* + 1/2; (iv) -*x* + 1, *y* + 1/2, -*z* + 1/2; (v) *x*, *y* + 1, *z*.]

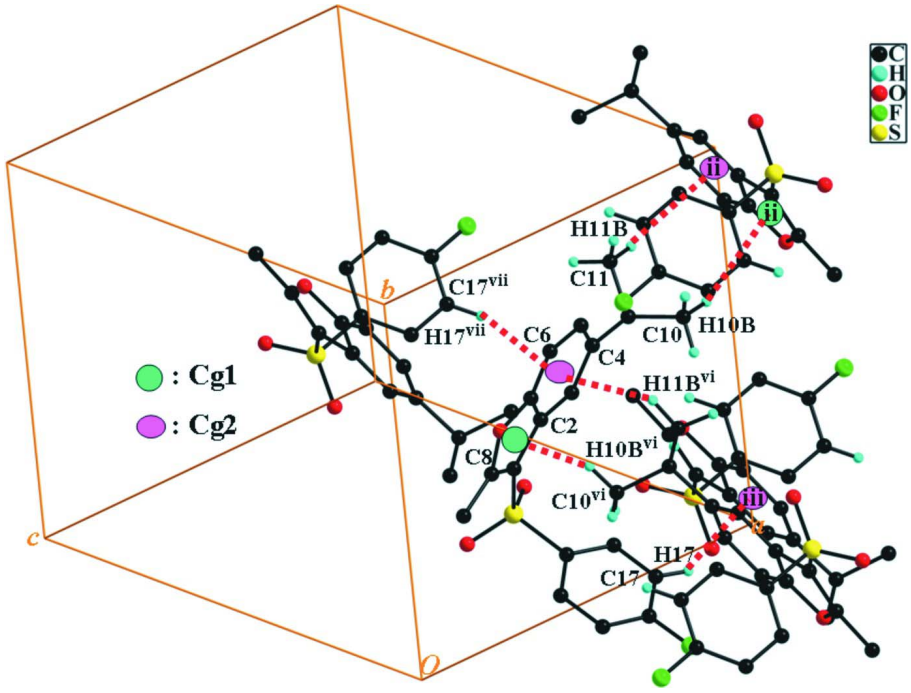


**Figure 3**

C—H···$\pi$ interactions (dotted lines) in the crystal structure of the title compound. Cg denotes the ring centroid. [Symmetry codes: (ii) -$x$ + 2, $y$ + 1/2, -$z$ + 1/2; (iii) $x$, -$y$ + 1/2, $z$ - 1/2; (vi) -$x$ + 2, $y$ - 1/2, -$z$ + 1/2; (vii) $x$, -$y$ + 1/2, $z$ + 1/2.]

### 3-(4-Fluorophenylsulfonyl)-5-isopropyl-2-methyl-1-benzofuran

*Crystal data*

$C_{18}H_{17}FO_3S$
$M_r$ = 332.38
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 10.9434 (6) Å
$b$ = 11.3395 (6) Å
$c$ = 13.0988 (7) Å
$\beta$ = 100.252 (3)°
$V$ = 1599.51 (15) Å$^3$
$Z$ = 4
$F(000)$ = 696
$D_x$ = 1.380 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 6367 reflections
$\theta$ = 2.4–27.5°
$\mu$ = 0.23 mm$^{-1}$
$T$ = 175 K
Block, colourless
0.41 × 0.29 × 0.17 mm

*Data collection*

Bruker SMART APEXII CCD diffractometer
Radiation source: rotating anode
Graphite multilayer monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.669, $T_{max}$ = 0.746
14304 measured reflections
3655 independent reflections
3109 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.030
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.4°
$h$ = −14→14
$k$ = −14→14
$l$ = −16→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.108$
$S = 1.02$
3655 reflections
212 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
$w = 1/[\sigma^2(F_o^2) + (0.0594P)^2 + 0.4509P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å$^{-3}$
$\Delta\rho_{min} = -0.37$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0117 (15)

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S | 0.54221 (3) | 0.13196 (3) | 0.21925 (3) | 0.02922 (13) |
| F | 0.75485 (9) | −0.21439 (9) | −0.02852 (8) | 0.0475 (3) |
| O1 | 0.44396 (10) | 0.07695 (11) | 0.26153 (9) | 0.0415 (3) |
| O2 | 0.51752 (10) | 0.23800 (9) | 0.15885 (8) | 0.0367 (3) |
| O3 | 0.79447 (10) | 0.15165 (9) | 0.47328 (8) | 0.0300 (2) |
| C1 | 0.66335 (13) | 0.16383 (12) | 0.32124 (11) | 0.0268 (3) |
| C2 | 0.75540 (12) | 0.25570 (12) | 0.32202 (10) | 0.0244 (3) |
| C3 | 0.78117 (13) | 0.34256 (12) | 0.25361 (11) | 0.0270 (3) |
| H3 | 0.7288 | 0.3527 | 0.1881 | 0.032* |
| C4 | 0.88480 (13) | 0.41423 (13) | 0.28261 (11) | 0.0285 (3) |
| C5 | 0.96004 (13) | 0.39900 (13) | 0.38020 (11) | 0.0302 (3) |
| H5 | 1.0300 | 0.4491 | 0.3993 | 0.036* |
| C6 | 0.93628 (13) | 0.31367 (13) | 0.44994 (11) | 0.0297 (3) |
| H6 | 0.9877 | 0.3038 | 0.5159 | 0.036* |
| C7 | 0.83340 (13) | 0.24398 (12) | 0.41752 (10) | 0.0257 (3) |
| C8 | 0.69246 (14) | 0.10323 (13) | 0.41204 (11) | 0.0303 (3) |
| C9 | 0.91774 (15) | 0.50549 (14) | 0.20723 (12) | 0.0356 (4) |
| H9 | 0.8483 | 0.5073 | 0.1462 | 0.043* |
| C10 | 1.0351 (2) | 0.47032 (18) | 0.16761 (16) | 0.0548 (5) |
| H10A | 1.1061 | 0.4728 | 0.2249 | 0.082* |
| H10B | 1.0492 | 0.5253 | 0.1132 | 0.082* |
| H10C | 1.0256 | 0.3902 | 0.1392 | 0.082* |
| C11 | 0.9299 (2) | 0.62926 (15) | 0.25374 (16) | 0.0531 (5) |

| | | | | |
|---|---|---|---|---|
| H11A | 0.8558 | 0.6477 | 0.2832 | 0.080* |
| H11B | 0.9381 | 0.6866 | 0.1994 | 0.080* |
| H11C | 1.0036 | 0.6329 | 0.3085 | 0.080* |
| C12 | 0.64435 (18) | −0.00464 (15) | 0.45463 (14) | 0.0452 (4) |
| H12A | 0.5675 | −0.0294 | 0.4094 | 0.068* |
| H12B | 0.6275 | 0.0117 | 0.5243 | 0.068* |
| H12C | 0.7062 | −0.0677 | 0.4584 | 0.068* |
| C13 | 0.60386 (13) | 0.02725 (12) | 0.14291 (11) | 0.0274 (3) |
| C14 | 0.60321 (15) | −0.09153 (13) | 0.16991 (12) | 0.0342 (3) |
| H14 | 0.5684 | −0.1159 | 0.2279 | 0.041* |
| C15 | 0.65382 (15) | −0.17364 (14) | 0.11133 (13) | 0.0375 (4) |
| H15 | 0.6546 | −0.2551 | 0.1283 | 0.045* |
| C16 | 0.70315 (14) | −0.13427 (13) | 0.02763 (13) | 0.0332 (3) |
| C17 | 0.70304 (14) | −0.01834 (14) | −0.00155 (12) | 0.0344 (3) |
| H17 | 0.7364 | 0.0049 | −0.0606 | 0.041* |
| C18 | 0.65300 (14) | 0.06423 (13) | 0.05734 (12) | 0.0309 (3) |
| H18 | 0.6523 | 0.1454 | 0.0394 | 0.037* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S | 0.0237 (2) | 0.0283 (2) | 0.0349 (2) | −0.00195 (13) | 0.00319 (14) | −0.00717 (14) |
| F | 0.0421 (6) | 0.0428 (6) | 0.0595 (7) | 0.0017 (4) | 0.0145 (5) | −0.0195 (5) |
| O1 | 0.0295 (6) | 0.0473 (7) | 0.0503 (7) | −0.0098 (5) | 0.0138 (5) | −0.0133 (5) |
| O2 | 0.0336 (6) | 0.0308 (6) | 0.0412 (6) | 0.0052 (4) | −0.0057 (5) | −0.0056 (5) |
| O3 | 0.0344 (6) | 0.0300 (5) | 0.0254 (5) | −0.0011 (4) | 0.0047 (4) | 0.0015 (4) |
| C1 | 0.0263 (7) | 0.0248 (7) | 0.0296 (7) | −0.0011 (5) | 0.0061 (5) | −0.0042 (5) |
| C2 | 0.0238 (6) | 0.0237 (7) | 0.0254 (7) | 0.0010 (5) | 0.0033 (5) | −0.0044 (5) |
| C3 | 0.0282 (7) | 0.0272 (7) | 0.0238 (7) | −0.0006 (5) | 0.0001 (5) | −0.0015 (5) |
| C4 | 0.0309 (7) | 0.0270 (7) | 0.0280 (7) | −0.0026 (6) | 0.0060 (6) | −0.0031 (6) |
| C5 | 0.0276 (7) | 0.0305 (7) | 0.0317 (8) | −0.0043 (6) | 0.0032 (6) | −0.0058 (6) |
| C6 | 0.0299 (7) | 0.0317 (7) | 0.0253 (7) | 0.0021 (6) | −0.0009 (5) | −0.0044 (6) |
| C7 | 0.0296 (7) | 0.0248 (7) | 0.0229 (7) | 0.0026 (5) | 0.0055 (5) | −0.0014 (5) |
| C8 | 0.0318 (7) | 0.0298 (7) | 0.0307 (8) | −0.0016 (6) | 0.0096 (6) | −0.0033 (6) |
| C9 | 0.0429 (9) | 0.0341 (8) | 0.0288 (7) | −0.0112 (7) | 0.0035 (6) | 0.0009 (6) |
| C10 | 0.0683 (13) | 0.0476 (11) | 0.0569 (12) | −0.0131 (9) | 0.0341 (10) | −0.0023 (9) |
| C11 | 0.0834 (14) | 0.0304 (9) | 0.0503 (11) | −0.0054 (9) | 0.0247 (10) | 0.0037 (8) |
| C12 | 0.0516 (10) | 0.0413 (9) | 0.0444 (10) | −0.0111 (8) | 0.0130 (8) | 0.0077 (8) |
| C13 | 0.0245 (7) | 0.0263 (7) | 0.0302 (7) | −0.0030 (5) | 0.0023 (5) | −0.0041 (6) |
| C14 | 0.0398 (8) | 0.0281 (7) | 0.0351 (8) | −0.0050 (6) | 0.0080 (6) | −0.0006 (6) |
| C15 | 0.0423 (9) | 0.0249 (7) | 0.0445 (9) | −0.0006 (6) | 0.0054 (7) | −0.0022 (7) |
| C16 | 0.0248 (7) | 0.0340 (8) | 0.0396 (9) | −0.0004 (6) | 0.0029 (6) | −0.0126 (6) |
| C17 | 0.0315 (8) | 0.0378 (8) | 0.0349 (8) | −0.0083 (6) | 0.0087 (6) | −0.0040 (6) |
| C18 | 0.0303 (7) | 0.0269 (7) | 0.0350 (8) | −0.0057 (6) | 0.0046 (6) | −0.0004 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S—O1 | 1.437 (1) | C9—C11 | 1.526 (2) |
| S—O2 | 1.438 (1) | C9—H9 | 1.0000 |
| S—C1 | 1.744 (2) | C10—H10A | 0.9800 |
| S—C13 | 1.762 (1) | C10—H10B | 0.9800 |
| F—C16 | 1.355 (2) | C10—H10C | 0.9800 |
| O3—C8 | 1.368 (2) | C11—H11A | 0.9800 |
| O3—C7 | 1.386 (2) | C11—H11B | 0.9800 |
| C1—C8 | 1.361 (2) | C11—H11C | 0.9800 |
| C1—C2 | 1.448 (2) | C12—H12A | 0.9800 |
| C2—C7 | 1.390 (2) | C12—H12B | 0.9800 |
| C2—C3 | 1.394 (2) | C12—H12C | 0.9800 |
| C3—C4 | 1.392 (2) | C13—C14 | 1.393 (2) |
| C3—H3 | 0.9500 | C13—C18 | 1.391 (2) |
| C4—C5 | 1.403 (2) | C14—C15 | 1.383 (2) |
| C4—C9 | 1.517 (2) | C14—H14 | 0.9500 |
| C5—C6 | 1.387 (2) | C15—C16 | 1.380 (2) |
| C5—H5 | 0.9500 | C15—H15 | 0.9500 |
| C6—C7 | 1.379 (2) | C16—C17 | 1.369 (2) |
| C6—H6 | 0.9500 | C17—C18 | 1.386 (2) |
| C8—C12 | 1.480 (2) | C17—H17 | 0.9500 |
| C9—C10 | 1.521 (2) | C18—H18 | 0.9500 |
| | | | |
| O1—S—O2 | 119.66 (7) | C9—C10—H10A | 109.5 |
| O1—S—C1 | 108.28 (7) | C9—C10—H10B | 109.5 |
| O2—S—C1 | 106.91 (7) | H10A—C10—H10B | 109.5 |
| O1—S—C13 | 108.33 (7) | C9—C10—H10C | 109.5 |
| O2—S—C13 | 107.74 (7) | H10A—C10—H10C | 109.5 |
| C1—S—C13 | 104.99 (7) | H10B—C10—H10C | 109.5 |
| C8—O3—C7 | 106.82 (11) | C9—C11—H11A | 109.5 |
| C8—C1—C2 | 107.62 (13) | C9—C11—H11B | 109.5 |
| C8—C1—S | 126.33 (11) | H11A—C11—H11B | 109.5 |
| C2—C1—S | 125.97 (11) | C9—C11—H11C | 109.5 |
| C7—C2—C3 | 118.96 (12) | H11A—C11—H11C | 109.5 |
| C7—C2—C1 | 104.63 (12) | H11B—C11—H11C | 109.5 |
| C3—C2—C1 | 136.39 (13) | C8—C12—H12A | 109.5 |
| C4—C3—C2 | 119.04 (13) | C8—C12—H12B | 109.5 |
| C4—C3—H3 | 120.5 | H12A—C12—H12B | 109.5 |
| C2—C3—H3 | 120.5 | C8—C12—H12C | 109.5 |
| C3—C4—C5 | 119.64 (13) | H12A—C12—H12C | 109.5 |
| C3—C4—C9 | 119.80 (13) | H12B—C12—H12C | 109.5 |
| C5—C4—C9 | 120.53 (13) | C14—C13—C18 | 121.08 (14) |
| C6—C5—C4 | 122.53 (13) | C14—C13—S | 119.19 (11) |
| C6—C5—H5 | 118.7 | C18—C13—S | 119.73 (11) |
| C4—C5—H5 | 118.7 | C15—C14—C13 | 119.29 (14) |
| C7—C6—C5 | 115.82 (13) | C15—C14—H14 | 120.4 |
| C7—C6—H6 | 122.1 | C13—C14—H14 | 120.4 |

| | | | |
|---|---|---|---|
| C5—C6—H6 | 122.1 | C16—C15—C14 | 118.36 (14) |
| C6—C7—O3 | 125.53 (13) | C16—C15—H15 | 120.8 |
| C6—C7—C2 | 124.01 (13) | C14—C15—H15 | 120.8 |
| O3—C7—C2 | 110.45 (12) | F—C16—C17 | 118.17 (14) |
| C1—C8—O3 | 110.44 (13) | F—C16—C15 | 118.35 (14) |
| C1—C8—C12 | 134.67 (15) | C17—C16—C15 | 123.48 (14) |
| O3—C8—C12 | 114.75 (13) | C16—C17—C18 | 118.29 (14) |
| C4—C9—C10 | 110.85 (14) | C16—C17—H17 | 120.9 |
| C4—C9—C11 | 112.42 (13) | C18—C17—H17 | 120.9 |
| C10—C9—C11 | 110.99 (15) | C17—C18—C13 | 119.49 (14) |
| C4—C9—H9 | 107.4 | C17—C18—H18 | 120.3 |
| C10—C9—H9 | 107.4 | C13—C18—H18 | 120.3 |
| C11—C9—H9 | 107.4 | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14···O2$^{i}$ | 0.95 | 2.51 | 3.401 (2) | 155 |
| C10—H10*B*···*Cg*1$^{ii}$ | 0.98 | 2.86 | 3.561 (2) | 120 |
| C11—H11*B*···*Cg*2$^{ii}$ | 0.98 | 2.91 | 3.670 (2) | 135 |
| C17—H17···*Cg*2$^{iii}$ | 0.95 | 2.89 | 3.528 (2) | 147 |

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