# organic compounds

# 5-(4-Fluorophenyl)-3-methylsulfanyl-2-phenyl-1-benzofuran

## Hong Dae Choi,[a] Pil Ja Seo,[a] Byeng Wha Son[b] and Uk Lee[b]*

[a]Department of Chemistry, Dongeui University, San 24 Kaya-dong Busanjin-gu, Busan 614-714, Republic of Korea, and [b]Department of Chemistry, Pukyong National University, 599-1 Daeyeon 3-dong, Nam-gu, Busan 608-737, Republic of Korea

Correspondence e-mail: uklee@pknu.ac.kr

In the title compound, $C_{21}H_{15}FOS$, the dihedral angle between the mean plane of the benzofuran fragment and the mean planes of the pendant 4-fluorobenzene and phenyl rings are 31.72 (6)° and 32.51 (6)°, respectively. In the crystal, the molecules are linked by weak C—H⋯$\pi$ interactions. The crystal studied was a merohedral twin with a 0.62 (9):0.38 (9) domain ratio.

## Related literature

For background to the pharmacological activity of benzofuran compounds, see: Aslam *et al.* (2009); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For structural studies of 2-(4-halophenyl)-3-methylsulfanyl-5-phenyl-1-benzofuran drivatives, see: Choi *et al.* (2009, 2010).
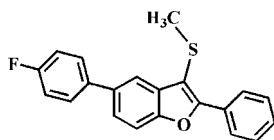


## Experimental

### Crystal data

| | |
|---|---|
| $C_{21}H_{15}FOS$ | $a = 10.6439$ (15) Å |
| $M_r = 334.39$ | $b = 7.2006$ (10) Å |
| Monoclinic, $P2_1$ | $c = 11.7226$ (17) Å |
| $\beta = 115.396$ (2)° | $\mu = 0.21$ mm$^{-1}$ |
| $V = 811.6$ (2) Å$^3$ | $T = 173$ K |
| $Z = 2$ | $0.36 \times 0.29 \times 0.10$ mm |
| Mo $K\alpha$ radiation | |

### Data collection

| | |
|---|---|
| Bruker SMART APEXII CCD diffractometer | 7372 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | 3194 independent reflections |
| | 2540 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.928$, $T_{max} = 0.979$ | $R_{int} = 0.035$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | H-atom parameters constrained |
| $wR(F^2) = 0.106$ | $\Delta\rho_{max} = 0.21$ e Å$^{-3}$ |
| $S = 1.10$ | $\Delta\rho_{min} = -0.20$ e Å$^{-3}$ |
| 3194 reflections | Absolute structure: Flack (1983), 1278 Friedel pairs |
| 219 parameters | Flack parameter: 0.38 (9) |
| 1 restraint | |

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

$Cg$ is the centroid of the C15–C20 phenyl ring.

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C14—H14⋯$Cg^i$ | 0.95 | 2.76 | 3.448 (2) | 130 |

Symmetry code: (i) $-x+1, y+\frac{3}{2}, -z+1$.

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* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

## 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., Son, B. W. & Lee, U. (2009). *Acta Cryst.* E**65**, o2766.
Choi, H. D., Seo, P. J., Son, B. W. & Lee, U. (2010). *Acta Cryst.* E**66**, o802.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Galal, S. A., Abd El-All, A. S., Abdallah, M. M. & El-Diwani, H. I. (2009). *Bioorg. Med. Chem. Lett.* **19**, 2420–2428.
Khan, M. W., Alam, M. J., Rashid, M. A. & Chowdhury, R. (2005). *Bioorg. Med. Chem.* **13**, 4796–4805.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Soekamto, N. H., Achmad, S. A., Ghisalberti, E. L., Hakim, E. H. & Syah, Y. M. (2003). *Phytochemistry*, **64**, 831–834.

**supplementary materials**

## 5-(4-Fluorophenyl)-3-methylsulfanyl-2-phenyl-1-benzofuran

### H. D. Choi, P. J. Seo, B. W. Son and U. Lee

### Comment

Recently, many compounds having a benzofuran moiety have drawn much attention due to their valuable pharmacological properties such as antibacterial and antifungal, antitumor and antiviral, and antimicrobial activities (Aslam *et al.*, 2009, Galal *et al.*, 2009, Khan *et al.*, 2005). These benzofuran derivatives occur in a wide range of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing studies of the substituent effect on the solid state structures of 2-(4-halophenyl)-3-methylsulfanyl-5-phenyl-1-benzofuran analogues (Choi *et al.*, 2009, 2010), we report herein the crystal structure of the title compound.

The title compound crystallizes as the non-centrosymmetric space group $P2_1$ in spite of having no asymmetric C atoms. The crystal studied was an inversion twin with a 0.68 (9) : 0.32 (9) domain ratio.

In the title molecule (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.006 (2) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle formed by the 4-fluorophenyl ring and the mean plane of the benzofurn fragment is 31.72 (6)°. The dihedral angle between the phenyl ring and the mean plane of the benzofurn fragment is 32.51 (6)°. The crystal packing (Fig. 2) is stabilized by intermolecular C—H···π interactions between a 4-fluorophenyl H atom and the phenyl ring (Table 1; C14—H14···Cg[i], Cg is the centroid of the C15–C20 phenyl ring).

### Experimental

Zinc chloride (273 mg, 2.0 mmol) was added to a stirred solution of 4-fluoro-4'-hydroxybiphenyl (376 mg, 2.0 mmol) and 2-chloro-2-methylsulfanylacetophenone (401 mg, 2.0 mmol) in dichloromethane (30 mL) at room temperature, and stirring was continued at the same temperature for 1 h. The reaction was quenched by the addition of water and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated at reduced pressure. The residue was purified by column chromatography (hexane–benzene, 5:2 v/v) to afford the title compound as a colorless solid [yield 61%, m.p. 415–416 K; $R_f$ = 0.78 (hexane–benzene, 5:2 v/v)]. Colourless blocks were prepared by slow evaporation of a solution of the title compound in carbon tetrachloride at room temperature.

### Refinement

The reported Flack parameter was obtained by TWIN/BASF procedure in SHELXL (Sheldrick, 2008). 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. $U_{iso}(H) = 1.2U_{eq}(C)$ for aryl and $1.5U_{eq}(C)$ for methyl H atoms.
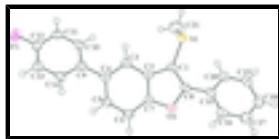
# supplementary materials

**Figures**



Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.
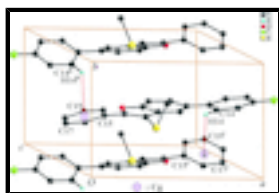


Fig. 2. A view of the C—H⋯π interactions (dotted lines) in the crystal structure of the title compound. Symmetry codes: (i) - $x$ + 1, $y$ - 1/2, - $z$ + 1; (ii) - $x$ + 1, $y$ + 1/2, - $z$ + 1.]

## 5-(4-Fluorophenyl)-3-methylsulfanyl-2-phenyl-1-benzofuran

*Crystal data*

| | |
|---|---|
| $C_{21}H_{15}FOS$ | $F(000) = 348$ |
| $M_r = 334.39$ | $D_x = 1.368$ Mg m$^{-3}$ |
| Monoclinic, $P2_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2yb | Cell parameters from 2652 reflections |
| $a = 10.6439$ (15) Å | $\theta = 3.4–26.6°$ |
| $b = 7.2006$ (10) Å | $\mu = 0.21$ mm$^{-1}$ |
| $c = 11.7226$ (17) Å | $T = 173$ K |
| $\beta = 115.396$ (2)° | Block, colourless |
| $V = 811.6$ (2) Å$^3$ | $0.36 \times 0.29 \times 0.10$ mm |
| $Z = 2$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD diffractometer | 3194 independent reflections |
| Radiation source: rotating anode | 2540 reflections with $I > 2\sigma(I)$ |
| graphite multilayer | $R_{int} = 0.035$ |
| Detector resolution: 10.0 pixels mm$^{-1}$ | $\theta_{max} = 27.0°$, $\theta_{min} = 1.9°$ |
| φ and ω scans | $h = -12 \rightarrow 13$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $k = -8 \rightarrow 9$ |
| $T_{min} = 0.928$, $T_{max} = 0.979$ | $l = -14 \rightarrow 14$ |
| 7372 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | H-atom parameters constrained |
| $wR(F^2) = 0.106$ | $w = 1/[\sigma^2(F_o^2) + (0.0545P)^2]$ |

where $P = (F_o^2 + 2F_c^2)/3$

| | |
|---|---|
| $S = 1.10$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 3194 reflections | $\Delta\rho_{max} = 0.21$ e Å$^{-3}$ |
| 219 parameters | $\Delta\rho_{min} = -0.20$ e Å$^{-3}$ |
| 1 restraint | Absolute structure: Flack (1983), 1278 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.38 (9) |

*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 | 0.42262 (6) | 0.39699 (11) | 0.12213 (5) | 0.03595 (18) |
| F1 | 1.34923 (15) | 0.4759 (3) | 0.74321 (14) | 0.0487 (4) |
| O1 | 0.34169 (16) | 0.4817 (2) | 0.41757 (13) | 0.0299 (4) |
| C1 | 0.4191 (2) | 0.4505 (3) | 0.26649 (19) | 0.0269 (5) |
| C2 | 0.5384 (2) | 0.4604 (3) | 0.38747 (19) | 0.0259 (5) |
| C3 | 0.6812 (2) | 0.4542 (3) | 0.42791 (19) | 0.0280 (5) |
| H3 | 0.7195 | 0.4416 | 0.3685 | 0.034* |
| C4 | 0.7681 (2) | 0.4667 (3) | 0.5565 (2) | 0.0272 (5) |
| C5 | 0.7074 (3) | 0.4836 (4) | 0.6427 (2) | 0.0306 (5) |
| H5 | 0.7670 | 0.4914 | 0.7303 | 0.037* |
| C6 | 0.5661 (3) | 0.4890 (4) | 0.6047 (2) | 0.0327 (6) |
| H6 | 0.5269 | 0.4998 | 0.6635 | 0.039* |
| C7 | 0.4842 (2) | 0.4781 (4) | 0.47627 (19) | 0.0273 (5) |
| C8 | 0.3042 (2) | 0.4667 (3) | 0.28925 (19) | 0.0272 (5) |
| C9 | 0.9222 (2) | 0.4655 (3) | 0.60428 (19) | 0.0264 (5) |
| C10 | 0.9871 (3) | 0.5412 (3) | 0.5334 (2) | 0.0294 (5) |
| H10 | 0.9317 | 0.5924 | 0.4526 | 0.035* |
| C11 | 1.1301 (3) | 0.5429 (3) | 0.5785 (2) | 0.0307 (5) |
| H11 | 1.1734 | 0.5928 | 0.5294 | 0.037* |
| C12 | 1.2080 (2) | 0.4703 (4) | 0.6967 (2) | 0.0329 (5) |
| C13 | 1.1500 (2) | 0.3955 (4) | 0.7699 (2) | 0.0330 (5) |
| H13 | 1.2067 | 0.3478 | 0.8515 | 0.040* |
| C14 | 1.0067 (2) | 0.3910 (4) | 0.72242 (18) | 0.0290 (5) |
| H14 | 0.9648 | 0.3359 | 0.7712 | 0.035* |
| C15 | 0.1550 (2) | 0.4714 (3) | 0.2092 (2) | 0.0274 (5) |

| | | | | |
|---|---|---|---|---|
| C16 | 0.0615 (2) | 0.4006 (4) | 0.25293 (19) | 0.0312 (5) |
| H16 | 0.0956 | 0.3464 | 0.3346 | 0.037* |
| C17 | −0.0797 (3) | 0.4087 (4) | 0.1787 (2) | 0.0373 (6) |
| H17 | −0.1424 | 0.3593 | 0.2090 | 0.045* |
| C18 | −0.1305 (3) | 0.4888 (4) | 0.0595 (2) | 0.0383 (6) |
| H18 | −0.2278 | 0.4939 | 0.0082 | 0.046* |
| C19 | −0.0387 (3) | 0.5614 (4) | 0.0158 (2) | 0.0359 (6) |
| H19 | −0.0736 | 0.6180 | −0.0651 | 0.043* |
| C20 | 0.1025 (3) | 0.5520 (3) | 0.0887 (2) | 0.0316 (5) |
| H20 | 0.1646 | 0.6002 | 0.0573 | 0.038* |
| C21 | 0.4698 (4) | 0.6154 (6) | 0.0774 (3) | 0.0679 (11) |
| H21A | 0.3992 | 0.7088 | 0.0688 | 0.102* |
| H21B | 0.4756 | 0.6015 | −0.0033 | 0.102* |
| H21C | 0.5602 | 0.6553 | 0.1425 | 0.102* |

*Atomic displacement parameters ($Å^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0428 (4) | 0.0435 (3) | 0.0252 (2) | 0.0018 (3) | 0.0181 (2) | −0.0041 (3) |
| F1 | 0.0285 (9) | 0.0664 (11) | 0.0510 (9) | −0.0028 (8) | 0.0168 (7) | 0.0080 (8) |
| O1 | 0.0319 (9) | 0.0355 (8) | 0.0257 (7) | 0.0000 (8) | 0.0157 (6) | −0.0012 (7) |
| C1 | 0.0348 (13) | 0.0234 (11) | 0.0242 (10) | 0.0000 (10) | 0.0143 (9) | −0.0008 (8) |
| C2 | 0.0336 (13) | 0.0234 (10) | 0.0236 (9) | 0.0006 (10) | 0.0152 (9) | −0.0005 (8) |
| C3 | 0.0348 (13) | 0.0264 (11) | 0.0271 (10) | 0.0023 (10) | 0.0175 (9) | −0.0009 (9) |
| C4 | 0.0334 (13) | 0.0216 (9) | 0.0287 (10) | −0.0003 (11) | 0.0152 (9) | −0.0002 (9) |
| C5 | 0.0336 (14) | 0.0354 (12) | 0.0225 (10) | −0.0029 (11) | 0.0117 (10) | −0.0021 (9) |
| C6 | 0.0386 (15) | 0.0375 (14) | 0.0282 (11) | −0.0013 (12) | 0.0204 (10) | −0.0037 (10) |
| C7 | 0.0253 (13) | 0.0301 (11) | 0.0281 (11) | 0.0002 (11) | 0.0130 (9) | −0.0002 (9) |
| C8 | 0.0362 (13) | 0.0251 (10) | 0.0224 (9) | 0.0001 (11) | 0.0144 (9) | 0.0016 (8) |
| C9 | 0.0324 (14) | 0.0223 (10) | 0.0280 (10) | −0.0022 (11) | 0.0162 (10) | −0.0031 (9) |
| C10 | 0.0371 (15) | 0.0270 (11) | 0.0250 (10) | −0.0001 (10) | 0.0142 (10) | 0.0011 (9) |
| C11 | 0.0354 (15) | 0.0297 (12) | 0.0338 (12) | −0.0021 (11) | 0.0213 (11) | 0.0003 (10) |
| C12 | 0.0273 (14) | 0.0327 (12) | 0.0400 (12) | −0.0026 (12) | 0.0157 (10) | −0.0038 (11) |
| C13 | 0.0309 (13) | 0.0363 (12) | 0.0305 (10) | 0.0000 (13) | 0.0119 (9) | 0.0017 (11) |
| C14 | 0.0339 (13) | 0.0289 (10) | 0.0281 (9) | −0.0041 (12) | 0.0170 (9) | 0.0024 (11) |
| C15 | 0.0315 (13) | 0.0221 (10) | 0.0289 (10) | 0.0027 (11) | 0.0131 (9) | −0.0017 (9) |
| C16 | 0.0389 (14) | 0.0256 (10) | 0.0321 (10) | 0.0011 (12) | 0.0181 (10) | 0.0023 (11) |
| C17 | 0.0392 (14) | 0.0305 (13) | 0.0449 (12) | −0.0061 (12) | 0.0208 (11) | −0.0044 (12) |
| C18 | 0.0296 (14) | 0.0326 (14) | 0.0441 (14) | 0.0015 (12) | 0.0076 (11) | −0.0083 (11) |
| C19 | 0.0436 (17) | 0.0294 (13) | 0.0266 (11) | 0.0027 (12) | 0.0073 (11) | −0.0005 (9) |
| C20 | 0.0387 (15) | 0.0273 (12) | 0.0303 (11) | −0.0009 (11) | 0.0162 (11) | 0.0000 (9) |
| C21 | 0.091 (3) | 0.073 (2) | 0.0554 (19) | −0.026 (2) | 0.047 (2) | 0.0069 (16) |

*Geometric parameters ($Å$, °)*

| | | | |
|---|---|---|---|
| S1—C1 | 1.752 (2) | C10—H10 | 0.9500 |
| S1—C21 | 1.796 (3) | C11—C12 | 1.377 (3) |
| F1—C12 | 1.362 (3) | C11—H11 | 0.9500 |
| O1—C7 | 1.371 (3) | C12—C13 | 1.365 (3) |

| | | | |
|---|---|---|---|
| O1—C8 | 1.385 (2) | C13—C14 | 1.382 (3) |
| C1—C8 | 1.364 (3) | C13—H13 | 0.9500 |
| C1—C2 | 1.444 (3) | C14—H14 | 0.9500 |
| C2—C3 | 1.385 (3) | C15—C16 | 1.397 (3) |
| C2—C7 | 1.396 (3) | C15—C20 | 1.402 (3) |
| C3—C4 | 1.393 (3) | C16—C17 | 1.378 (3) |
| C3—H3 | 0.9500 | C16—H16 | 0.9500 |
| C4—C5 | 1.418 (3) | C17—C18 | 1.388 (4) |
| C4—C9 | 1.489 (3) | C17—H17 | 0.9500 |
| C5—C6 | 1.374 (4) | C18—C19 | 1.385 (4) |
| C5—H5 | 0.9500 | C18—H18 | 0.9500 |
| C6—C7 | 1.381 (3) | C19—C20 | 1.376 (3) |
| C6—H6 | 0.9500 | C19—H19 | 0.9500 |
| C8—C15 | 1.458 (3) | C20—H20 | 0.9500 |
| C9—C14 | 1.395 (3) | C21—H21A | 0.9800 |
| C9—C10 | 1.399 (3) | C21—H21B | 0.9800 |
| C10—C11 | 1.380 (3) | C21—H21C | 0.9800 |
| | | | |
| C1—S1—C21 | 102.33 (13) | C10—C11—H11 | 120.9 |
| C7—O1—C8 | 106.56 (16) | F1—C12—C13 | 118.6 (2) |
| C8—C1—C2 | 106.77 (18) | F1—C12—C11 | 118.5 (2) |
| C8—C1—S1 | 126.90 (17) | C13—C12—C11 | 122.9 (2) |
| C2—C1—S1 | 125.83 (17) | C12—C13—C14 | 118.4 (2) |
| C3—C2—C7 | 119.45 (19) | C12—C13—H13 | 120.8 |
| C3—C2—C1 | 135.12 (19) | C14—C13—H13 | 120.8 |
| C7—C2—C1 | 105.4 (2) | C13—C14—C9 | 121.4 (2) |
| C2—C3—C4 | 119.4 (2) | C13—C14—H14 | 119.3 |
| C2—C3—H3 | 120.3 | C9—C14—H14 | 119.3 |
| C4—C3—H3 | 120.3 | C16—C15—C20 | 118.8 (2) |
| C3—C4—C5 | 118.9 (2) | C16—C15—C8 | 120.38 (19) |
| C3—C4—C9 | 121.32 (19) | C20—C15—C8 | 120.8 (2) |
| C5—C4—C9 | 119.82 (19) | C17—C16—C15 | 120.6 (2) |
| C6—C5—C4 | 122.8 (2) | C17—C16—H16 | 119.7 |
| C6—C5—H5 | 118.6 | C15—C16—H16 | 119.7 |
| C4—C5—H5 | 118.6 | C16—C17—C18 | 120.1 (2) |
| C5—C6—C7 | 116.3 (2) | C16—C17—H17 | 119.9 |
| C5—C6—H6 | 121.8 | C18—C17—H17 | 119.9 |
| C7—C6—H6 | 121.8 | C19—C18—C17 | 119.8 (2) |
| O1—C7—C6 | 126.3 (2) | C19—C18—H18 | 120.1 |
| O1—C7—C2 | 110.47 (18) | C17—C18—H18 | 120.1 |
| C6—C7—C2 | 123.3 (2) | C20—C19—C18 | 120.5 (2) |
| C1—C8—O1 | 110.74 (19) | C20—C19—H19 | 119.8 |
| C1—C8—C15 | 134.14 (19) | C18—C19—H19 | 119.8 |
| O1—C8—C15 | 115.12 (19) | C19—C20—C15 | 120.2 (2) |
| C14—C9—C10 | 117.8 (2) | C19—C20—H20 | 119.9 |
| C14—C9—C4 | 120.84 (19) | C15—C20—H20 | 119.9 |
| C10—C9—C4 | 121.3 (2) | S1—C21—H21A | 109.5 |
| C11—C10—C9 | 121.4 (2) | S1—C21—H21B | 109.5 |
| C11—C10—H10 | 119.3 | H21A—C21—H21B | 109.5 |
| C9—C10—H10 | 119.3 | S1—C21—H21C | 109.5 |

| | | | |
|---|---|---|---|
| C12—C11—C10 | 118.1 (2) | H21A—C21—H21C | 109.5 |
| C12—C11—H11 | 120.9 | H21B—C21—H21C | 109.5 |
| C21—S1—C1—C8 | 107.9 (3) | C3—C4—C9—C14 | −149.0 (2) |
| C21—S1—C1—C2 | −81.3 (2) | C5—C4—C9—C14 | 31.9 (3) |
| C8—C1—C2—C3 | −179.5 (3) | C3—C4—C9—C10 | 31.9 (3) |
| S1—C1—C2—C3 | 8.2 (4) | C5—C4—C9—C10 | −147.2 (2) |
| C8—C1—C2—C7 | 1.3 (3) | C14—C9—C10—C11 | −0.2 (4) |
| S1—C1—C2—C7 | −171.00 (18) | C4—C9—C10—C11 | 178.9 (2) |
| C7—C2—C3—C4 | −0.3 (3) | C9—C10—C11—C12 | −0.9 (3) |
| C1—C2—C3—C4 | −179.4 (3) | C10—C11—C12—F1 | −178.3 (2) |
| C2—C3—C4—C5 | 0.6 (3) | C10—C11—C12—C13 | 0.7 (4) |
| C2—C3—C4—C9 | −178.4 (2) | F1—C12—C13—C14 | 179.7 (2) |
| C3—C4—C5—C6 | −0.3 (4) | C11—C12—C13—C14 | 0.7 (4) |
| C9—C4—C5—C6 | 178.8 (2) | C12—C13—C14—C9 | −1.9 (4) |
| C4—C5—C6—C7 | −0.3 (4) | C10—C9—C14—C13 | 1.7 (4) |
| C8—O1—C7—C6 | −179.9 (2) | C4—C9—C14—C13 | −177.4 (2) |
| C8—O1—C7—C2 | −0.2 (3) | C1—C8—C15—C16 | 148.6 (3) |
| C5—C6—C7—O1 | −179.7 (2) | O1—C8—C15—C16 | −31.5 (3) |
| C5—C6—C7—C2 | 0.7 (4) | C1—C8—C15—C20 | −33.4 (4) |
| C3—C2—C7—O1 | 180.0 (2) | O1—C8—C15—C20 | 146.6 (2) |
| C1—C2—C7—O1 | −0.7 (3) | C20—C15—C16—C17 | 0.4 (4) |
| C3—C2—C7—C6 | −0.3 (4) | C8—C15—C16—C17 | 178.5 (3) |
| C1—C2—C7—C6 | 179.0 (2) | C15—C16—C17—C18 | −0.5 (4) |
| C2—C1—C8—O1 | −1.5 (3) | C16—C17—C18—C19 | −0.3 (4) |
| S1—C1—C8—O1 | 170.70 (16) | C17—C18—C19—C20 | 1.0 (4) |
| C2—C1—C8—C15 | 178.5 (2) | C18—C19—C20—C15 | −1.1 (4) |
| S1—C1—C8—C15 | −9.3 (4) | C16—C15—C20—C19 | 0.3 (4) |
| C7—O1—C8—C1 | 1.1 (3) | C8—C15—C20—C19 | −177.7 (2) |
| C7—O1—C8—C15 | −178.9 (2) | | |

*Hydrogen-bond geometry (Å, °)*

Cg is the centroid of the C15–C20 phenyl ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14···Cg^i | 0.95 | 2.76 | 3.448 (2) | 130 |

Symmetry codes: (i) −*x*+1, *y*+3/2, −*z*+1.

**Fig. 1**

**Fig. 2**