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1-Methyl-2-({[(2-methylphenyl)methyl]-disulfanylmethyl)benzene

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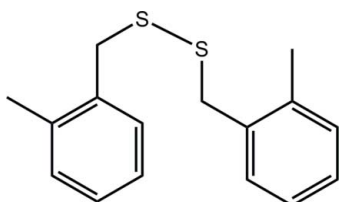
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 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.035; wR factor = 0.096; data-to-parameter ratio = 16.8.

In the title disulfide, $\text{C}_{16}\text{H}_{18}\text{S}_2$, the molecule is twisted about the central S—S bond [the C—S—S—C torsion angle = $93.24(7)^\circ$] and the dihedral angle between the benzene rings is $72.84(7)^\circ$, indicating an almost orthogonal relationship; the methyl groups are orientated to the same side of the molecule. The crystal packing features C—H $\cdots\pi$ interactions which consolidate a three-dimensional architecture.

Related literature

For background to the coordination chemistry of dithiocarbamate derivatives, see: Crouse *et al.* (2004); Ravoof *et al.* (2010). For the synthesis and methodology, see: Tarafder *et al.* (2000). For the structure of bis(benzyl)disulfide, see: van Dijk & Visser (1971).



Experimental

Crystal data

 $\text{C}_{16}\text{H}_{18}\text{S}_2$
 $M_r = 274.42$
 Monoclinic, $P2_1/c$
 $a = 10.3640(4)$ Å
 $b = 7.6408(3)$ Å
 $c = 18.1106(7)$ Å
 $\beta = 91.099(3)^\circ$
 $V = 1433.90(10)$ Å³
 $Z = 4$
 Cu $K\alpha$ radiation
 $\mu = 3.18$ mm⁻¹
 $T = 100$ K
 $0.56 \times 0.38 \times 0.21$ mm

Data collection

 Oxford Diffraction Xcalibur Eos
 Gemini diffractometer
 Absorption correction: multi-scan
 (*CrysAlis PRO*; Agilent, 2011)
 $T_{\min} = 0.299$, $T_{\max} = 0.513$
 9993 measured reflections
 2773 independent reflections
 2672 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.096$
 $S = 1.06$
 2773 reflections
 165 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.41$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C2–C7 and C10–C15 rings, respectively.

| D—H \cdots A | D—H | H \cdots A | D \cdots A | D—H \cdots A |
|--------------------------------------|------|--------------|--------------|----------------|
| C1—H1B \cdots Cg1 ⁱ | 0.99 | 2.91 | 3.4605 (16) | 116 |
| C16—H16B \cdots Cg2 ⁱⁱ | 0.98 | 2.85 | 3.7392 (18) | 151 |
| C16—H16C \cdots Cg1 ⁱⁱⁱ | 0.98 | 2.97 | 3.7764 (18) | 140 |

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

Data collection: *CrysAlis PRO* (Agilent, 2011); 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: *publCIF* (Westrip, 2010).

Support for the project came from Universiti Putra Malaysia (UPM) through the purchase of the diffractometer and under their Research University Grant Scheme (RUGS No. 9174000), the Malaysian Ministry of Science, Technology and Innovation (grant No. 09-02-04-0752-EA001) and the Malaysian Fundamental Research Grant Scheme (FRGS No. 01-13-11-986FR). The authors also thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (UM.C/HIR/MOHE/SC/12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6818).

References

- Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.
- Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Crouse, K. A., Chew, K. B., Tarafder, M. T. H., Kasbollah, A., Ali, M. A., Yamin, B. M. & Fun, H.-K. (2004). *Polyhedron*, **23**, 161–168.
- Dijk, B. van & Visser, G. J. (1971). *Acta Cryst.* **B27**, 846.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Ravoof, T. B. S. A., Crouse, K. A., Tahir, M. I. M., How, F. N. F., Rosli, R. & Watkins, D. J. (2010). *Transition Met. Chem.* **35**, 871–876.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Tarafder, M. T. H., Ali, M. A., Wee, D. J., Azahari, K., Silong, S. & Crouse, K. A. (2000). *Transition Met. Chem.* **25**, 456–460.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

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1-Methyl-2-([(2-methylphenyl)methyl]disulfanyl)methyl)benzene

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S1. Comment

Our interest in investigating the coordination properties of ligands containing the H—N—C=S moiety and our desire to expand the study of this class of biologically important compounds has lead us to synthesize series of related ligands (Tarafder *et al.*, 2000; Crouse *et al.*, 2004; Ravoof *et al.*, 2010). The title compound, [(2-methyl)benzyl]disulfide, (I), was obtained during the attempt to prepare the phenyl hydrazine analogue of *S*-benzylidithiocarbazate.

In (I), Fig. 1, the molecule is twisted about the central S1—S2 bond as seen in the value of the C1—S1—S2—C9 torsion angle of 93.24 (7) Å. The dihedral between the benzene rings is 72.84 (7)°, indicating an almost orthogonal relationship, and the methyl groups are orientated to the same side of the molecule. The overall conformation in (I) contrasts that found in the parent compound, bis(benzyl)disulfide (van Dijk & Visser, 1971), which adopts an open conformation with both phenyl rings directed away from the sulfur atoms. In (I), the S1-bound benzyl is directed away having an *anti* disposition [the S2—S1—C1—C2 torsion angle is 176.23 (9)°] whereas the S2-bound benzyl residue in bis(benzyl)disulfide (van Dijk & Visser, 1971) has a *syn* conformation [S1—C1—C2—C7 = 91.90 (14)°].

The crystal packing is dominated by C—H... π interactions, Table 1, which consolidates a three-dimensional architecture, Fig. 2.

S2. Experimental

[(2-Methyl)benzyl]disulfide was isolated as a by-product from the synthesis of the phenylhydrazine analog of *S*-benzylidithiocarbazate (Tarafder *et al.*, 2000). Potassium hydroxide (0.2 mol, 11.2 g) was completely dissolved in absolute ethanol (70 ml) and phenylhydrazine (0.2 mol, 21.6 g) was added to the solution cooled in an ice-salt bath producing a dark-yellow solution. Carbon disulfide (0.2 mol, 15.2 g) was added drop-wise with constant stirring over one hour. 2-Methylbenzyl chloride (0.1 mol, 13.2 ml) was then added drop-wise with vigorous stirring. The temperature of reaction was maintained below 278 K. The high yield yellow-white product was filtered and dried in a dessicator over anhydrous silica gel, dissolved in absolute ethanol and kept in a freezer. A few colourless blocks were harvested on the third day and washed with cold n-hexane.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H = 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation with $U_{\text{iso}}(\text{H})$ set to 1.2 to 1.5 $U_{\text{equiv}}(\text{C})$.

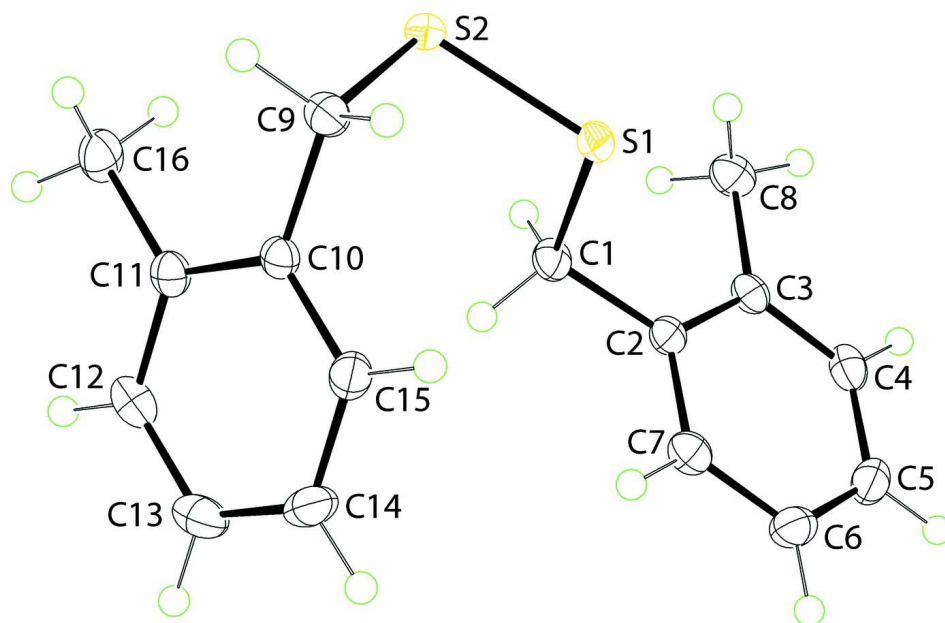


Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

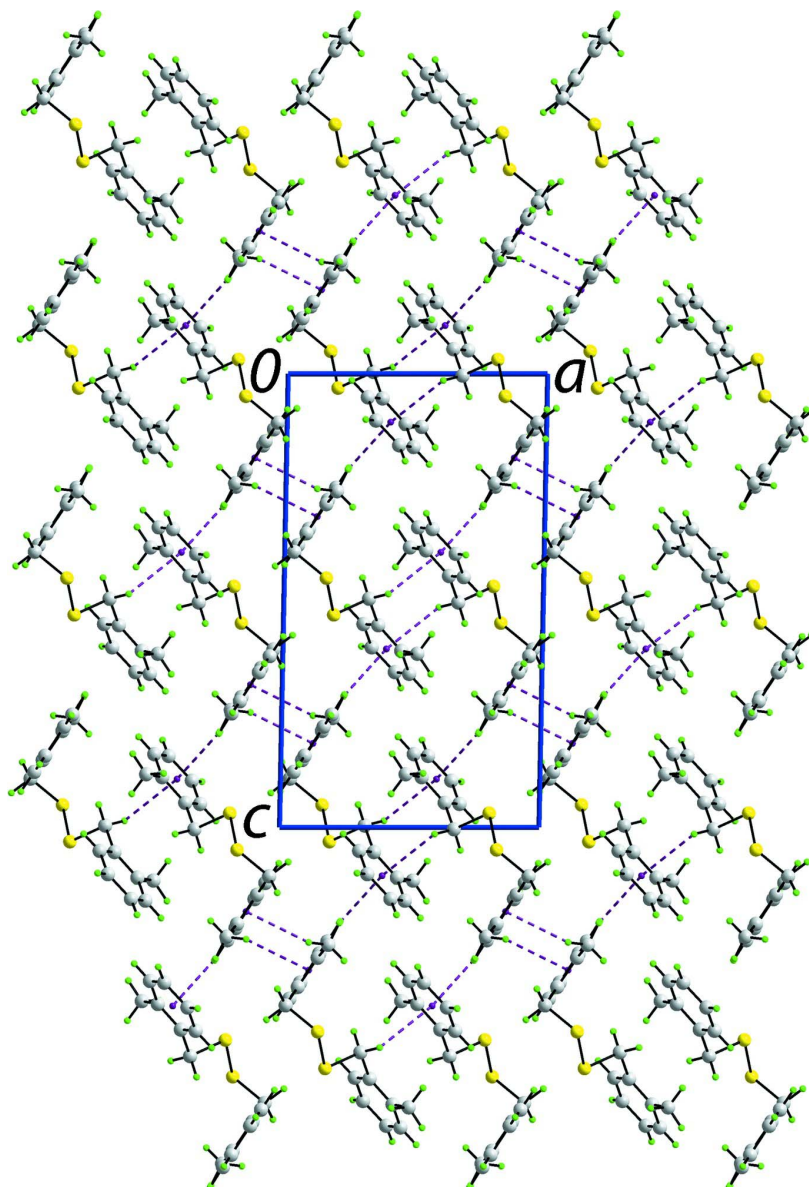


Figure 2

A view in projection down the b axis of the unit-cell contents for (I). The C—H \cdots π interactions are shown as purple dashed lines.

1-Methyl-2-([(2-methylphenyl)methyl]disulfanyl)methylbenzene

Crystal data

$C_{16}H_{18}S_2$

$M_r = 274.42$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 10.3640(4)\ \text{\AA}$

$b = 7.6408(3)\ \text{\AA}$

$c = 18.1106(7)\ \text{\AA}$

$\beta = 91.099(3)^\circ$

$V = 1433.90(10)\ \text{\AA}^3$

$Z = 4$

$F(000) = 584$

$D_x = 1.271\ \text{Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54180\ \text{\AA}$

Cell parameters from 5536 reflections

$\theta = 4\text{--}71^\circ$

$\mu = 3.18\ \text{mm}^{-1}$

$T = 100$ K $0.56 \times 0.38 \times 0.21$ mm
 Block, colourless

Data collection

| | |
|---|--|
| Oxford Diffraction Xcalibur Eos Gemini diffractometer | 9993 measured reflections |
| Radiation source: fine-focus sealed tube | 2773 independent reflections |
| Graphite monochromator | 2672 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 16.1952 pixels mm ⁻¹ | $R_{\text{int}} = 0.023$ |
| ω scans | $\theta_{\text{max}} = 71.6^\circ$, $\theta_{\text{min}} = 4.3^\circ$ |
| Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2011) | $h = -12 \rightarrow 12$ |
| $T_{\text{min}} = 0.299$, $T_{\text{max}} = 0.513$ | $k = -8 \rightarrow 9$ |
| | $l = -21 \rightarrow 22$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.035$ | H-atom parameters constrained |
| $wR(F^2) = 0.096$ | $w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.5578P]$ |
| $S = 1.06$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 2773 reflections | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 165 parameters | $\Delta\rho_{\text{max}} = 0.41 \text{ e } \text{\AA}^{-3}$ |
| 0 restraints | $\Delta\rho_{\text{min}} = -0.22 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | |

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|-------------|---------------|----------------------------------|
| S1 | 0.19303 (3) | 0.79536 (5) | 0.531391 (19) | 0.01839 (13) |
| S2 | 0.16204 (3) | 0.97650 (5) | 0.450468 (19) | 0.01857 (13) |
| C1 | 0.32793 (14) | 0.6661 (2) | 0.49591 (8) | 0.0197 (3) |
| H1A | 0.3014 | 0.6058 | 0.4497 | 0.024* |
| H1B | 0.4019 | 0.7435 | 0.4853 | 0.024* |
| C2 | 0.36554 (14) | 0.5340 (2) | 0.55430 (8) | 0.0175 (3) |
| C3 | 0.45586 (14) | 0.5739 (2) | 0.61072 (8) | 0.0190 (3) |
| C4 | 0.48816 (15) | 0.4427 (2) | 0.66150 (8) | 0.0231 (3) |
| H4 | 0.5498 | 0.4670 | 0.6996 | 0.028* |
| C5 | 0.43266 (16) | 0.2782 (2) | 0.65765 (9) | 0.0252 (4) |
| H5 | 0.4571 | 0.1908 | 0.6925 | 0.030* |
| C6 | 0.34159 (17) | 0.2409 (2) | 0.60306 (10) | 0.0254 (3) |
| H6 | 0.3022 | 0.1287 | 0.6007 | 0.030* |
| C7 | 0.30838 (15) | 0.3688 (2) | 0.55173 (8) | 0.0216 (3) |

| | | | | |
|------|--------------|--------------|--------------|------------|
| H7 | 0.2457 | 0.3434 | 0.5143 | 0.026* |
| C8 | 0.51809 (16) | 0.7523 (2) | 0.61716 (10) | 0.0258 (4) |
| H8A | 0.5715 | 0.7574 | 0.6623 | 0.039* |
| H8B | 0.4509 | 0.8424 | 0.6191 | 0.039* |
| H8C | 0.5722 | 0.7729 | 0.5742 | 0.039* |
| C9 | 0.03670 (14) | 0.8731 (2) | 0.39237 (8) | 0.0197 (3) |
| H9A | -0.0361 | 0.8389 | 0.4239 | 0.024* |
| H9B | 0.0039 | 0.9600 | 0.3561 | 0.024* |
| C10 | 0.08223 (14) | 0.71442 (19) | 0.35152 (8) | 0.0168 (3) |
| C11 | 0.15632 (14) | 0.7299 (2) | 0.28736 (8) | 0.0187 (3) |
| C12 | 0.19310 (14) | 0.5778 (2) | 0.25128 (9) | 0.0232 (3) |
| H12 | 0.2407 | 0.5869 | 0.2071 | 0.028* |
| C13 | 0.16219 (16) | 0.4131 (2) | 0.27805 (9) | 0.0265 (4) |
| H13 | 0.1895 | 0.3111 | 0.2528 | 0.032* |
| C14 | 0.09121 (16) | 0.3982 (2) | 0.34191 (10) | 0.0262 (4) |
| H14 | 0.0706 | 0.2861 | 0.3610 | 0.031* |
| C15 | 0.05054 (15) | 0.5485 (2) | 0.37768 (9) | 0.0209 (3) |
| H15 | 0.0002 | 0.5382 | 0.4208 | 0.025* |
| C16 | 0.19659 (16) | 0.9069 (2) | 0.25888 (9) | 0.0263 (4) |
| H16A | 0.2582 | 0.9603 | 0.2939 | 0.039* |
| H16B | 0.1205 | 0.9822 | 0.2534 | 0.039* |
| H16C | 0.2373 | 0.8930 | 0.2108 | 0.039* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|---------------|---------------|---------------|
| S1 | 0.0218 (2) | 0.0188 (2) | 0.0146 (2) | 0.00273 (13) | 0.00327 (14) | -0.00021 (12) |
| S2 | 0.0244 (2) | 0.0138 (2) | 0.0175 (2) | -0.00018 (13) | -0.00079 (14) | -0.00113 (12) |
| C1 | 0.0196 (7) | 0.0225 (8) | 0.0173 (7) | 0.0042 (6) | 0.0039 (5) | -0.0003 (6) |
| C2 | 0.0176 (7) | 0.0187 (8) | 0.0164 (7) | 0.0027 (6) | 0.0046 (5) | -0.0009 (5) |
| C3 | 0.0176 (7) | 0.0222 (8) | 0.0175 (7) | 0.0020 (6) | 0.0036 (5) | -0.0031 (6) |
| C4 | 0.0223 (7) | 0.0301 (9) | 0.0169 (7) | 0.0060 (6) | 0.0009 (6) | -0.0017 (6) |
| C5 | 0.0297 (8) | 0.0245 (9) | 0.0217 (8) | 0.0077 (6) | 0.0065 (6) | 0.0058 (6) |
| C6 | 0.0290 (8) | 0.0188 (8) | 0.0285 (8) | -0.0014 (6) | 0.0074 (7) | 0.0007 (6) |
| C7 | 0.0206 (7) | 0.0231 (8) | 0.0211 (7) | 0.0001 (6) | 0.0019 (6) | -0.0029 (6) |
| C8 | 0.0257 (8) | 0.0254 (9) | 0.0263 (8) | -0.0030 (7) | -0.0003 (6) | -0.0047 (7) |
| C9 | 0.0194 (7) | 0.0202 (8) | 0.0194 (7) | 0.0015 (6) | -0.0010 (5) | -0.0025 (6) |
| C10 | 0.0167 (7) | 0.0182 (8) | 0.0155 (7) | 0.0006 (5) | -0.0024 (5) | -0.0006 (5) |
| C11 | 0.0167 (7) | 0.0221 (8) | 0.0171 (7) | -0.0019 (6) | -0.0023 (5) | -0.0001 (6) |
| C12 | 0.0186 (7) | 0.0313 (9) | 0.0196 (7) | 0.0003 (6) | 0.0000 (6) | -0.0070 (6) |
| C13 | 0.0249 (8) | 0.0229 (9) | 0.0316 (9) | 0.0054 (6) | -0.0061 (6) | -0.0096 (7) |
| C14 | 0.0306 (8) | 0.0151 (8) | 0.0325 (9) | -0.0022 (6) | -0.0087 (7) | 0.0021 (6) |
| C15 | 0.0228 (7) | 0.0216 (8) | 0.0184 (7) | -0.0031 (6) | -0.0017 (6) | 0.0023 (6) |
| C16 | 0.0305 (8) | 0.0281 (9) | 0.0203 (8) | -0.0084 (7) | 0.0024 (6) | 0.0026 (6) |

Geometric parameters (Å, °)

| | | | |
|------------|-------------|--------------|-------------|
| S1—C1 | 1.8377 (15) | C8—H8C | 0.9800 |
| S1—S2 | 2.0368 (5) | C9—C10 | 1.501 (2) |
| S2—C9 | 1.8349 (15) | C9—H9A | 0.9900 |
| C1—C2 | 1.508 (2) | C9—H9B | 0.9900 |
| C1—H1A | 0.9900 | C10—C15 | 1.395 (2) |
| C1—H1B | 0.9900 | C10—C11 | 1.410 (2) |
| C2—C7 | 1.395 (2) | C11—C12 | 1.390 (2) |
| C2—C3 | 1.406 (2) | C11—C16 | 1.509 (2) |
| C3—C4 | 1.397 (2) | C12—C13 | 1.389 (3) |
| C3—C8 | 1.511 (2) | C12—H12 | 0.9500 |
| C4—C5 | 1.384 (2) | C13—C14 | 1.387 (3) |
| C4—H4 | 0.9500 | C13—H13 | 0.9500 |
| C5—C6 | 1.383 (3) | C14—C15 | 1.388 (2) |
| C5—H5 | 0.9500 | C14—H14 | 0.9500 |
| C6—C7 | 1.387 (2) | C15—H15 | 0.9500 |
| C6—H6 | 0.9500 | C16—H16A | 0.9800 |
| C7—H7 | 0.9500 | C16—H16B | 0.9800 |
| C8—H8A | 0.9800 | C16—H16C | 0.9800 |
| C8—H8B | 0.9800 | | |
| | | | |
| C1—S1—S2 | 102.94 (5) | H8B—C8—H8C | 109.5 |
| C9—S2—S1 | 102.71 (5) | C10—C9—S2 | 113.87 (10) |
| C2—C1—S1 | 107.61 (10) | C10—C9—H9A | 108.8 |
| C2—C1—H1A | 110.2 | S2—C9—H9A | 108.8 |
| S1—C1—H1A | 110.2 | C10—C9—H9B | 108.8 |
| C2—C1—H1B | 110.2 | S2—C9—H9B | 108.8 |
| S1—C1—H1B | 110.2 | H9A—C9—H9B | 107.7 |
| H1A—C1—H1B | 108.5 | C15—C10—C11 | 119.47 (14) |
| C7—C2—C3 | 119.79 (14) | C15—C10—C9 | 119.22 (14) |
| C7—C2—C1 | 118.60 (14) | C11—C10—C9 | 121.31 (13) |
| C3—C2—C1 | 121.61 (14) | C12—C11—C10 | 118.41 (14) |
| C4—C3—C2 | 118.07 (15) | C12—C11—C16 | 120.55 (14) |
| C4—C3—C8 | 120.01 (14) | C10—C11—C16 | 121.04 (14) |
| C2—C3—C8 | 121.92 (14) | C13—C12—C11 | 121.77 (15) |
| C5—C4—C3 | 121.66 (15) | C13—C12—H12 | 119.1 |
| C5—C4—H4 | 119.2 | C11—C12—H12 | 119.1 |
| C3—C4—H4 | 119.2 | C14—C13—C12 | 119.66 (15) |
| C4—C5—C6 | 120.03 (15) | C14—C13—H13 | 120.2 |
| C4—C5—H5 | 120.0 | C12—C13—H13 | 120.2 |
| C6—C5—H5 | 120.0 | C13—C14—C15 | 119.47 (15) |
| C5—C6—C7 | 119.40 (16) | C13—C14—H14 | 120.3 |
| C5—C6—H6 | 120.3 | C15—C14—H14 | 120.3 |
| C7—C6—H6 | 120.3 | C14—C15—C10 | 121.18 (15) |
| C6—C7—C2 | 121.02 (15) | C14—C15—H15 | 119.4 |
| C6—C7—H7 | 119.5 | C10—C15—H15 | 119.4 |
| C2—C7—H7 | 119.5 | C11—C16—H16A | 109.5 |

| | | | |
|-------------|--------------|-----------------|--------------|
| C3—C8—H8A | 109.5 | C11—C16—H16B | 109.5 |
| C3—C8—H8B | 109.5 | H16A—C16—H16B | 109.5 |
| H8A—C8—H8B | 109.5 | C11—C16—H16C | 109.5 |
| C3—C8—H8C | 109.5 | H16A—C16—H16C | 109.5 |
| H8A—C8—H8C | 109.5 | H16B—C16—H16C | 109.5 |
| <hr/> | | | |
| C1—S1—S2—C9 | 93.24 (7) | S1—S2—C9—C10 | -68.30 (11) |
| S2—S1—C1—C2 | 176.23 (9) | S2—C9—C10—C15 | 102.14 (14) |
| S1—C1—C2—C7 | 91.90 (14) | S2—C9—C10—C11 | -77.83 (16) |
| S1—C1—C2—C3 | -87.97 (15) | C15—C10—C11—C12 | 1.4 (2) |
| C7—C2—C3—C4 | 1.9 (2) | C9—C10—C11—C12 | -178.67 (13) |
| C1—C2—C3—C4 | -178.24 (13) | C15—C10—C11—C16 | -177.79 (14) |
| C7—C2—C3—C8 | -178.44 (14) | C9—C10—C11—C16 | 2.2 (2) |
| C1—C2—C3—C8 | 1.4 (2) | C10—C11—C12—C13 | -2.0 (2) |
| C2—C3—C4—C5 | -0.7 (2) | C16—C11—C12—C13 | 177.16 (14) |
| C8—C3—C4—C5 | 179.60 (15) | C11—C12—C13—C14 | 0.9 (2) |
| C3—C4—C5—C6 | -0.8 (2) | C12—C13—C14—C15 | 0.9 (2) |
| C4—C5—C6—C7 | 1.1 (2) | C13—C14—C15—C10 | -1.5 (2) |
| C5—C6—C7—C2 | 0.1 (2) | C11—C10—C15—C14 | 0.4 (2) |
| C3—C2—C7—C6 | -1.6 (2) | C9—C10—C15—C14 | -179.62 (14) |
| C1—C2—C7—C6 | 178.51 (14) | | |

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

Cg1 and Cg2 are the centroids of the C2—C7 and C10—C15 rings, respectively.

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|-------------------------------|-------------|---------------|-----------------------|-------------------------|
| C1—H1B...Cg1 ⁱ | 0.99 | 2.91 | 3.4605 (16) | 116 |
| C16—H16B...Cg2 ⁱⁱ | 0.98 | 2.85 | 3.7392 (18) | 151 |
| C16—H16C...Cg1 ⁱⁱⁱ | 0.98 | 2.97 | 3.7764 (18) | 140 |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, y+1/2, -z+1/2$; (iii) $x, -y+1/2, z-3/2$.