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2,5-Dimethyl-3,4-bis(methylsulfanyl)-7-phenylbenzo[1,2-*b*:4,3-*b*′]difuran

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-ku, Busan 614-714, Republic of Korea, and [b]Department of Chemistry, Pukyong National University, 599-1 Daeyeon 3-dong Nam-ku, Busan 608-737, Republic of Korea

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

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.060
wR factor = 0.126
Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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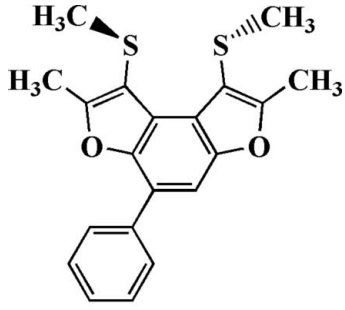
In the structure of the title compound, $C_{20}H_{18}O_2S_2$, the dihedral angle between the benzodifuran unit and the phenyl ring is 47.7 (1)°. In the crystal structure, some C—H bonds point in the direction of the centroids of the aromatic rings, which is indicative of C—H···π interactions.

Comment

The reported structure determination of the title compound, (I), was undertaken as part of our continuing studies of the syntheses and crystal structures of benzodifuran derivatives (Choi *et al.*, 2006).



(I)

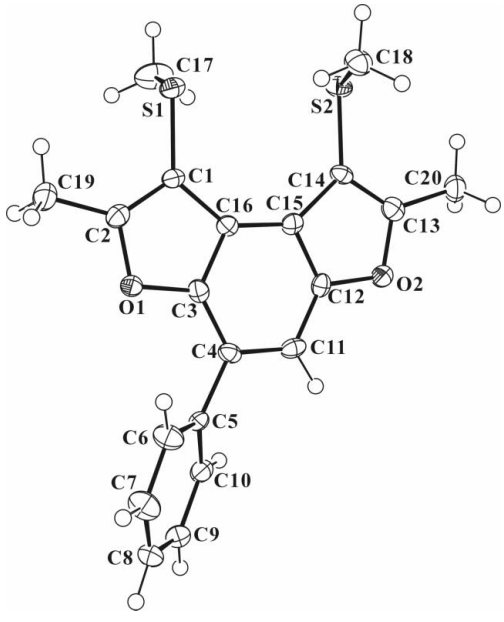


Figure 1
The molecular structure of (I), with labelling, and with displacement ellipsoids drawn at the 50% probability level for non–H atoms.

The benzo[1,2-*b*:4,3-*b*′]difuran ring system is nearly planar, with a mean deviation from the least-squares plane of 0.028 Å. The dihedral angle formed between the 7-phenyl ring and the benzodifuran unit is 47.7 (1)° (Fig. 1). In the crystal structure, some C—H bonds point in the direction of the aromatic rings, which is indicative of C—H···π interactions (Table 1; *Cg*1, *Cg*2 and *Cg*3 are the centroids of the C5–C10, C3/C4/C11/C12/C15/C16 and C1/C2/O1/C3/C16 rings, respectively).

Experimental

Zinc chloride (900 mg, 6.60 mmol) was added at room temperature to a stirred solution of phenylhydroquinone (559 mg, 3.0 mmol) and α-chloro-α-(methylsulfanyl)acetone (914 mg, 6.60 mmol) in dichloromethane (30 ml) and tetrahydrofuran (2 ml), and stirred for 40 min. The mixture was quenched with water and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (CCl_4) to afford (I) as a colourless solid. Crystals suitable for X-ray analysis were grown by slow evaporation of a carbon tetrachloride solution [yield 46%, m.p. 421–422 K; R_f = 0.64 (CCl_4)].

Crystal data

$C_{20}H_{18}O_2S_2$
M_r = 354.46
Monoclinic, $P2_1/c$
a = 10.0049 (7) Å
b = 7.8533 (6) Å
c = 21.880 (2) Å
β = 90.853 (1)°
V = 1719.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 173 (2) K
0.67 × 0.46 × 0.33 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
12247 measured reflections
3009 independent reflections
2632 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.126
S = 1.08
3009 reflections
221 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17*C*···*Cg*2^{i}	0.96	3.13	3.662 (5)	117
C18—H18*C*···*Cg*1^{ii}	0.96	2.85	3.772 (5)	162
C20—H20*A*···*Cg*3^{iii}	0.96	2.76	3.635 (5)	152

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

All H atoms were positioned with idealized geometry and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms, and with C—H = 0.93 Å for aromatic H atoms and 0.96 Å for methyl H atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

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