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2-Methyl-3-methylsulfinyl-5-phenyl-1-benzofuran

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.101
Data-to-parameter ratio = 16.4

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

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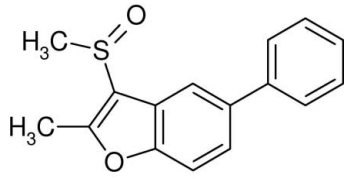
The title compound, $C_{16}H_{14}O_2S$, was prepared by oxidation of 2-methyl-3-methylsulfanyl-5-phenyl-1-benzofuran using 3-chloroperbenzoic acid. Short π–π stacking distances are prevented by the steric influence of the methylsulfinyl group.

Comment

1-Benzofuran compounds are important heterocyclic ring systems in the fields of natural product chemistry and medicinal chemistry because of their various pharmacological properties (Ward, 1997; Howlett *et al.*, 1999). The synthesis and reactivity of the 1-benzofuran ring has been widely investigated (Cagniant & Cagniant, 1975). As part of our continuing studies concerning the syntheses and structures of 1-benzofuran derivatives (Choi *et al.*, 2003, 2004; Choi, Seo *et al.*, 2006; Choi, Woo *et al.*, 2006), we report here the crystal structure of the title compound, (I), which was obtained by oxidation of 2-methyl-3-methylsulfanyl-5-phenyl-1-benzofuran using 3-chloroperbenzoic acid.



(I)

The bond lengths and angles in (I) are as expected for this type of compound (Choi, Seo *et al.*, 2006; Choi, Woo *et al.*, 2006). The dihedral angle formed between the phenyl ring and the benzofuran group is 31.89 (5)° (Fig. 1). The molecules are arranged into stacks with the planes of adjacent benzofuran groups approximately parallel, and with a separation of *ca* 4 Å between these planes. Shorter π–π stacking distances are prevented by the steric influence of the methylsulfinyl group.

Experimental

3-Chloroperbenzoic acid (77%, 471 mg, 2.1 mmol) was added in small portions to a stirred solution of 2-methyl-3-methylsulfanyl-5-phenyl-1-benzofuran (508 mg, 2.0 mmol) in dichloromethane (30 ml) at 273 K. After being stirred at room temperature for 1 h, the mixture was washed with saturated sodium bicarbonate solution. The organic layer was separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (EtOAc) to afford (I) as a white solid. Crystals suitable for X-ray analysis were obtained by slow evaporation of a chloroform solution [yield 86%, m.p. 390–391 K; R_F = 0.66 (EtOAc)].

Crystal data

$C_{16}H_{14}O_2S$
M_r = 270.33
Orthorhombic, *Pbcn*
a = 13.378 (1) Å
b = 7.8668 (6) Å
c = 24.931 (2) Å
V = 2623.8 (4) Å^3
Z = 8
D_x = 1.369 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 120 (2) K
Block, colourless
0.65 × 0.62 × 0.60 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: none
20982 measured reflections
2856 independent reflections
2480 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.101
S = 1.05
2856 reflections
174 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 1.2873P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

H atoms were placed geometrically and refined using a riding model, with C—H = 0.93 Å for aromatic and 0.96 Å for methyl H atoms, and with U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, and 1.5U_{eq}(C) for methyl H atoms. The methyl groups were allowed to rotate around their local threefold axes.

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); software used to prepare material for publication: *SHELXL97*.

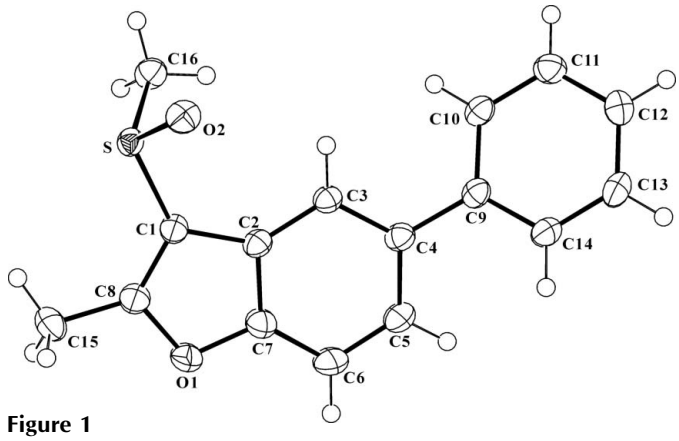


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level for non-H atoms.

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