Acta Crystallographica Section E
**Structure Reports**
**Online**
ISSN 1600-5368

# 2-Methyl-5,6-methylenedioxy-3-methylsulfinyl-1-benzofuran

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**Key indicators**

Single-crystal X-ray study
$T$ = 173 K
Mean $\sigma$(C–C) = 0.006 Å
$R$ factor = 0.095
$wR$ factor = 0.202
Data-to-parameter ratio = 15.5

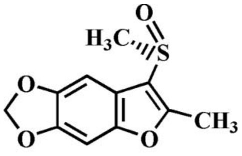
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 16 March 2007
Accepted 21 March 2007

The title compound, $C_{11}H_{10}O_4S$, was prepared by oxidation of 2-methyl-5,6-methylenedioxy-3-methylsulfanyl-1-benzofuran using 3-chloroperbenzoic acid. The 5,6-methylenedioxybenzofuran ring system is almost planar. The crystal structure contains aromatic $\pi-\pi$ stacking and $CH_2-H\cdots\pi$ interactions.

## Comment

This work is related to our previous communication on a 5,6-methylenedioxybenzofuran analogue (Choi, *et al.*, 2007), with the aim of understanding how the molecular conformation and crystal structure are affected by the methyl substituent. The title compound, (I) (Fig. 1), was obtained by oxidation of 2-methyl-5,6-methylenedioxy-3-methylsulfanyl-1-benzofuran with 3-chloroperbenzoic acid. The X-ray crystallographic analysis of this compound has been carried out and the results are presented here.



(I)

The bond lengths and angles in (I) are as expected for this type of compound (Choi *et al.*, 2007). The 5,6-methylenedioxybenzofuran unit is approximately planar, with a mean deviation of 0.020 Å from the least-squares plane defined by the 12 constituent atoms. In the crystal structure, $\pi$–$\pi$ stacking interactions are observed between the furan ring and the benzene ring of an adjacent benzofuran unit (Fig. 2). The $Cg1\cdots Cg2^{ii}$ distance is 3.981 (6) Å ($Cg1$ and $Cg2$ are the centroids of the O1/C9/C1/C2/C8 and C2–C4/ C6–C8 rings; symmetry code as in Fig. 2). C10—H10$B\cdots\pi$ interactions further stabilize the crystal structure (Table 1 and Fig. 2).

## Experimental

3-Chloroperbenzoic acid (77%, 314 mg, 1.40 mmol) was added in small portions to a stirred solution of 2-methyl-5,6-methylenedioxy-3-methylsulfanyl-1-benzofuran (289 mg, 1.30 mmol) in dichloromethane (20 ml) at 273 K. After stirring at room temperature for 1h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (ethyl acetate) to afford (I) as a white solid. Crystals suitable for X-ray analysis were grown by slow evaporation of a benzene solution [yield 81%, m.p. 407–408 K; $R_f$ = 0.31 (ethyl acetate)].

### *Crystal data*

$C_{11}H_{10}O_4S$
$M_r$ = 238.25
Monoclinic, $P2_1/n$
*a* = 5.0453 (5) Å
*b* = 12.642 (1) Å
*c* = 16.508 (2) Å
*β* = 95.556 (2)°

*V* = 1047.98 (18) Å$^3$
*Z* = 4
Mo *Kα* radiation
*μ* = 0.30 mm$^{-1}$
*T* = 173 (2) K
0.65 × 0.10 × 0.10 mm

### *Data collection*

Bruker SMART CCD diffractometer
Absorption correction: none
6212 measured reflections

2261 independent reflections
2023 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.093

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.095
$wR(F^2)$ = 0.202
*S* = 1.35
2261 reflections

146 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.67 e Å$^{-3}$
$\Delta\rho_{\rm min}$ = −0.46 e Å$^{-3}$

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

| *D*—H⋯*A* | *D*—H | H⋯*A* | *D*⋯*A* | *D*—H⋯*A* |
|---|---|---|---|---|
| C10—H10*B*⋯*Cg*1$^{i}$ | 0.96 | 2.93 | 3.841 (6) | 160 |

Symmetry code: (i) *x* − 1, *y*, *z*. *Cg*1 is the centroid of the O1/C9/C1/C2/C8.

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for aromatic H atoms and C—H = 0.96 Å for methyl H atoms, and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic H atoms, and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) 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* III (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

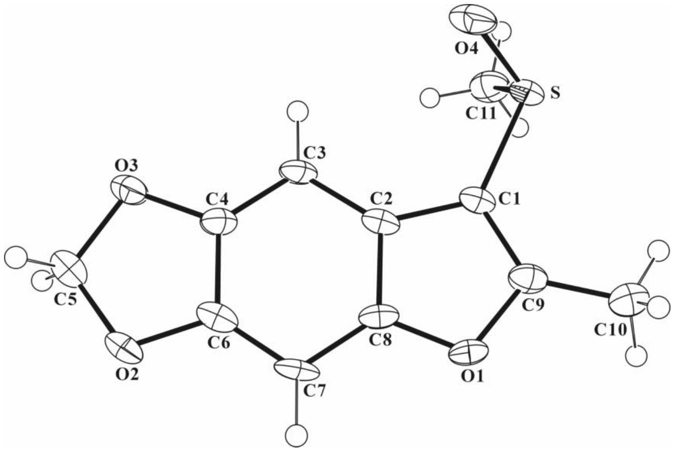


**Figure 1**
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level for non–H atoms.

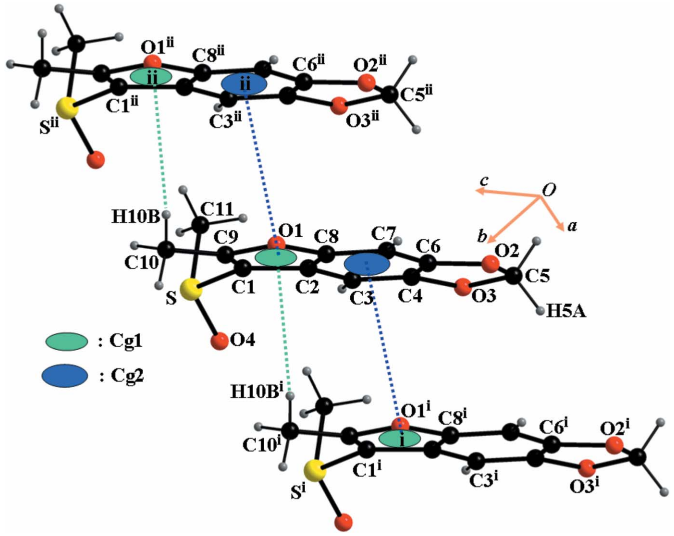


**Figure 2**
$\pi\cdots\pi$ and C—H⋯$\pi$ interactions (dotted lines) in (I). [Symmetry codes: (i) 1 + *x*, *y*, *z*; (ii) *x* − 1, *y*, *z*.]

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*Acta Cryst.* (2007). E**63**, o2050–o2051 Choi *et al.* • $C_{11}H_{10}O_4S$ **o2051**