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5-Bromo-2-methyl-3-methylsulfinylbenzofuran

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.005 Å
R factor = 0.052
wR factor = 0.152
Data-to-parameter ratio = 17.8

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

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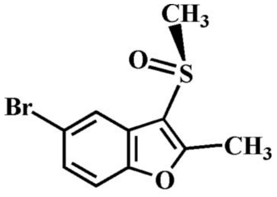
The title compound, $C_{10}H_9BrO_2S$, was prepared by the oxidation of 5-bromo-2-methyl-3-methylsulfanylbenzofuran using 3-chloroperbenzoic acid. The benzofuran ring system is almost planar. The crystal structure is stabilized by π–π stacking and –CH_2—H$\cdots\pi$ interactions.

Comment

As part of our ongoing investigations of benzofuran derivatives with interesting pharmacological activities (Choi *et al.*, 2003, 2006; Seo *et al.*, 2004), we report here the crystal structure of the title compound, (I) (Fig. 1), which was obtained by the oxidation of 5-bromo-2-methyl-3-methylsulfanylbenzofuran with 3-chloroperbenzoic acid. In (I), bond lengths and angles are as expected for this type of compound (Choi *et al.*, 2006) and the benzofuran unit is almost planar. In the crystal structure, molecules are arranged in stacks with the planes of adjacent benzofuran groups approximately parallel, and with a separation of 3.45 (2) Å between these planes. Shorter π–π stacking distances are prevented by the steric influence of the methylsulfinyl group.



(I)

The packing of the molecules (Fig. 2) is further stabilized by –CH_2—H$\cdots\pi$ interactions between the 2-methyl group and an adjacent furan ring, with a C9—H9$A\cdots Cg^{i}$ distance of 3.354 (5) Å (Cg is the centroid of the C4/C5/C7/C8/O1 ring; symmetry code as in Fig. 2).

Experimental

3-Chloroperbenzoic acid (77%, 471 mg, 2.10 mmol) was added in small portions to a stirred solution of 5-bromo-2-methyl-3-methylsulfanylbenzofuran (514 mg, 2.0 mmol) in dichloromethane (20 ml) at 273 K. After stirring at room temperature for 1 h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (ethyl acetate) to afford (I) as a colorless solid. Crystals suitable for X-ray analysis were grown by slow evaporation of an acetone solution [yield 84%; m.p. 418–419 K; R_f = 0.33 (ethyl acetate)].

Crystal data

$C_{10}H_9BrO_2S$
$M_r = 273.14$
Monoclinic, $P2_1/n$
$a = 5.2318\ (5)$ Å
$b = 16.466\ (2)$ Å
$c = 12.415\ (1)$ Å
$\beta = 94.846\ (2)^\circ$
$V = 1065.72\ (19)$ Å^3
$Z = 4$
$D_x = 1.702$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 4.02$ mm^{-1}
$T = 173\ (2)$ K
Needle, colorless
0.62 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1999)
$T_{\min} = 0.412$, $T_{\max} = 0.606$
5989 measured reflections
2292 independent reflections
1985 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.029$
$\theta_{\max} = 27.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.152$
$S = 1.01$
2292 reflections
129 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1094P)^2 + 1.0563P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.88$ e Å^{-3}
$\Delta\rho_{\min} = -1.60$ e Å^{-3}

All H atoms were geometrically located in ideal positions and refined using a riding model, with C—H = 0.93 Å, $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic and C—H = 0.96 Å, $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for CH_3 atoms. The highest peak in the difference map is 0.86 Å from Br and the largest hole is 0.82 Å from Br.

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*.

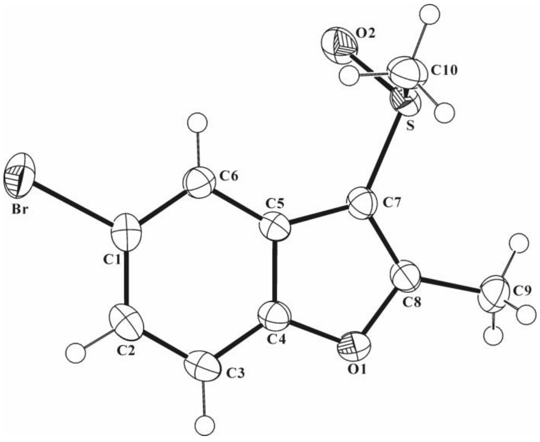


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level for non-H atoms.

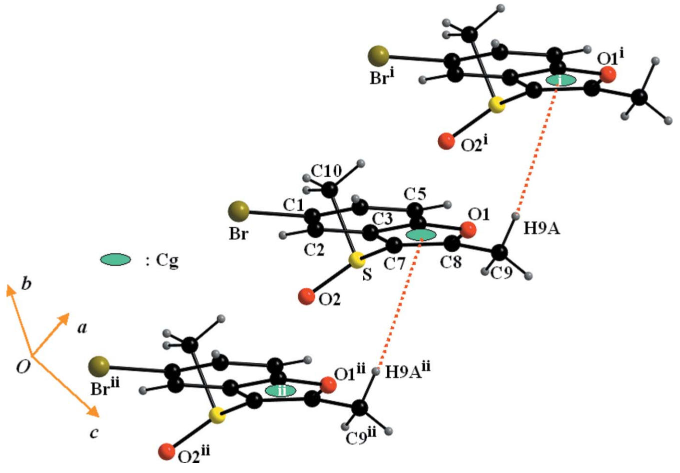


Figure 2
C—H$\cdots\pi$ interactions in (I). Green ellipses denote the centroids of the furan rings. [Symmetry codes: (i) $1 + x$, y, z; (ii) $x - 1$, y, z.]

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