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2-(4-Bromophenyl)-5,7-dimethyl-3-methylsulfinyl-1-benzofuran

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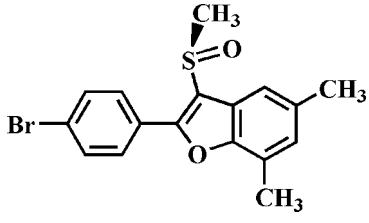
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.055; wR factor = 0.168; data-to-parameter ratio = 14.2.

The title compound, $C_{17}H_{15}BrO_2S$, was prepared by the oxidation of 2-(4-bromophenyl)-5,7-dimethyl-3-methylsulfanyl-1-benzofuran using 3-chloroperbenzoic acid. The 4-bromophenyl ring is rotated out of the benzofuran plane, with a dihedral angle of 19.3 (2)°. The O atom and the methyl group of the methylsulfinyl substituent lie on opposite sides of the plane of the benzofuran fragment. The crystal structure is stabilized by a C—H···O hydrogen bond, and a Br···O halogen bond with a Br···O distance of 3.209 (6)Å and a nearly linear C—Br···O angle of 165.1 (2)°.

Related literature

For crystal structures of isomers of the title compound, see: Choi *et al.* (2007*a*,*b*). For a review of halogen bonding, see: Politzer *et al.* (2007).



Experimental

Crystal data

$C_{17}H_{15}BrO_2S$
M_r = 363.26
Triclinic, $P\overline{1}$
a = 7.9802 (4) Å
b = 9.1652 (4) Å
c = 11.6042 (4) Å
α = 103.104 (3)°
β = 91.737 (3)°
γ = 106.648 (3)°
V = 787.84 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.74 mm^{-1}
T = 298 (2) K
0.24 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.519, T_{max} = 0.715
10316 measured reflections
2736 independent reflections
2061 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.168
S = 1.13
2736 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16A···O2^{i}	0.96	2.43	3.340 (10)	159

Symmetry code: (i) $x, y-1, z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2038).

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supplementary materials

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2-(4-Bromophenyl)-5,7-dimethyl-3-methylsulfinyl-1-benzofuran

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Comment

As part of our ongoing studies on the synthesis and structure of 2-aryl-5-methyl-3-methylsulfinyl-1-benzofuran analogues, we have recently described 5-methyl-3-methylsulfinyl-2-phenyl-1-benzofuran (Choi *et al.*, 2007*a*) and 2-(4-bromophenyl)-5-methyl-3-methylsulfinyl-1-benzofuran (Choi *et al.*, 2007*b*). Herein we report the molecular and crystal structure of the title compound, 2-(4-bromophenyl)-5,7-dimethyl-3-methylsulfinyl-1-benzofuran (Fig. 1).

The benzofuran unit is essentially planar, with a mean deviation of 0.014 Å from the least-squares plane defined by the nine constituent atoms. In the title compound, the dihedral angle between the plane of the benzofuran and the 4-bromophenyl ring is 19.3 (2)°. The molecular packing is stabilized by a C—H···O hydrogen bond; between a methyl H and the S═O unit, *i.e.* C16—H16A···O2^{i} (Table 1 & Fig. 2). The further stability comes from a weak C—Br···O halogen bond (Fig. 2) (Politzer *et al.*, 2007); between the bromine atom and the oxygen of a neighbouring S═O unit, *i.e.* C12—Br···O2^{ii} distance of 3.209 (6)Å and a nearly linear C—Br···O angle of 165.1 (2)Å (Symmetry codes as in Fig. 2).

Experimental

3-Chloroperbenzoic acid (77%, 359 mg, 1.60 mmol) was added in small portions to a stirred solution of 2-(4-bromophenyl)-5,7-dimethyl-3-methyl-sulfanyl-1-benzofuran (521 mg, 1.50 mmol) in dichloromethane (30 ml) at 273 K. After being stirred at room temperature for 2 h, 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 (hexane-ethyl acetate, 1:1 *v*/*v*) to afford the title compound as a colorless solid [yield 83%, m.p. 451–452 K; R_f = 0.65 (hexane-ethyl acetate, 1:1 *v*/*v*)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a dilute solution of the title compound in chloroform at room temperature.

Refinement

All H atoms were geometrically located in ideal positions and refined using a riding model, with C—H = 0.95 Å for aromatic H atoms and 0.98 Å for methyl H atoms, and with U_{iso}(H) = 1.2U_{eq}(C) for aromatic and 1.5Ueq(C) for methyl H atoms.

Figures

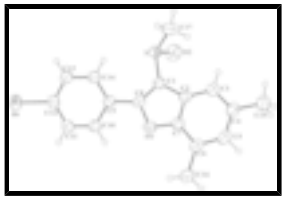

Fig. 1. The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level.

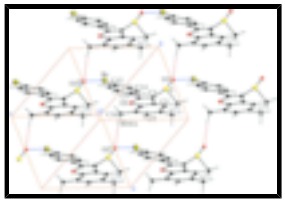

Fig. 2. The C—H···O hydrogen bond and Br···O halogen bond (dotted lines) in the title compound. [Symmetry code: (i) *x*, *y* − 1, *z*; (ii) *x*, *y*, *z* + 1.]

2-(4-Bromophenyl)-5,7-dimethyl-3-methylsulfinyl-1-benzofuran

Crystal data

$C_{17}H_{15}BrO_2S$	$Z = 2$
$M_r = 363.26$	$F_{000} = 368$
Triclinic, $P\overline{1}$	$D_x = 1.531$ Mg m^{-3}
Hall symbol: -p 1	Melting point: 451-452 K
$a = 7.9802$ (4) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 9.1652$ (4) Å	Cell parameters from 3012 reflections
$c = 11.6042$ (4) Å	$\theta = 2.6$–22.3°
$\alpha = 103.104$ (3)°	$\mu = 2.74$ mm^{-1}
$\beta = 91.737$ (3)°	$T = 298$ (2) K
$\gamma = 106.648$ (3)°	Block, colourless
$V = 787.84$ (6) Å^3	0.24 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer	2736 independent reflections
Radiation source: fine-focus sealed tube	2061 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.031$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 25.0^\circ$
$T = 298(2)$ K	$\theta_{min} = 1.8^\circ$
φ and ω scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (SADABS; Sheldrick, 2000)	$k = -10 \rightarrow 10$
$T_{min} = 0.519$, $T_{max} = 0.715$	$l = -12 \rightarrow 13$
10316 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.055$	H-atom parameters constrained
$wR(F^2) = 0.168$	$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 1.64P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} < 0.001$

2736 reflections	$\Delta\rho_{max} = 0.78$ e Å^{-3}
193 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br	0.24607 (10)	0.77634 (9)	0.54104 (6)	0.0801 (3)
S	0.4003 (2)	0.80276 (18)	−0.08002 (15)	0.0678 (5)
O1	0.1883 (5)	0.3767 (4)	−0.0363 (4)	0.0616 (10)
O2	0.2966 (8)	0.8282 (6)	−0.1757 (5)	0.0988 (17)
C1	0.3260 (7)	0.6002 (6)	−0.0870 (5)	0.0561 (14)
C2	0.2894 (7)	0.4718 (7)	−0.1935 (5)	0.0559 (14)
C3	0.3138 (8)	0.4579 (7)	−0.3137 (6)	0.0626 (15)
H3	0.3701	0.5454	−0.3411	0.075*
C4	0.2525 (8)	0.3116 (8)	−0.3901 (6)	0.0671 (16)
C5	0.1636 (8)	0.1822 (8)	−0.3474 (6)	0.0707 (18)
H5	0.1211	0.0849	−0.4015	0.085*
C6	0.1352 (8)	0.1907 (7)	−0.2292 (6)	0.0621 (15)
C7	0.2024 (7)	0.3401 (7)	−0.1565 (5)	0.0593 (14)
C8	0.2648 (7)	0.5352 (6)	0.0048 (5)	0.0555 (14)
C9	0.2613 (7)	0.5978 (7)	0.1328 (5)	0.0562 (14)
C10	0.1400 (8)	0.5092 (7)	0.1941 (6)	0.0626 (15)
H10	0.0624	0.4130	0.1534	0.075*
C11	0.1346 (8)	0.5633 (8)	0.3141 (6)	0.0636 (15)
H11	0.0548	0.5030	0.3545	0.076*
C12	0.2480 (8)	0.7075 (7)	0.3748 (5)	0.0601 (14)
C13	0.3688 (9)	0.7959 (8)	0.3167 (6)	0.0676 (16)
H13	0.4454	0.8923	0.3578	0.081*
C14	0.3755 (8)	0.7397 (7)	0.1955 (6)	0.0651 (16)
H14	0.4584	0.7988	0.1562	0.078*
C15	0.2770 (10)	0.2897 (10)	−0.5207 (6)	0.086 (2)
H15A	0.1642	0.2483	−0.5665	0.129*
H15B	0.3441	0.2178	−0.5429	0.129*
H15C	0.3383	0.3891	−0.5357	0.129*

C16	0.0351 (10)	0.0533 (8)	−0.1832 (7)	0.087 (2)
H16A	0.1152	0.0027	−0.1589	0.130*
H16B	−0.0507	−0.0201	−0.2448	0.130*
H16C	−0.0231	0.0897	−0.1163	0.130*
C17	0.6124 (10)	0.8137 (9)	−0.1298 (8)	0.093 (2)
H17A	0.6019	0.7284	−0.1979	0.139*
H17B	0.6892	0.8070	−0.0672	0.139*
H17C	0.6600	0.9117	−0.1510	0.139*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0910 (6)	0.0872 (5)	0.0626 (4)	0.0333 (4)	0.0112 (3)	0.0107 (3)
S	0.0821 (11)	0.0505 (8)	0.0690 (10)	0.0158 (8)	0.0107 (8)	0.0162 (7)
O1	0.059 (2)	0.053 (2)	0.069 (3)	0.0082 (18)	0.0044 (19)	0.018 (2)
O2	0.123 (4)	0.087 (4)	0.099 (4)	0.046 (3)	−0.008 (3)	0.034 (3)
C1	0.058 (3)	0.047 (3)	0.061 (3)	0.013 (3)	0.006 (3)	0.010 (3)
C2	0.049 (3)	0.051 (3)	0.066 (4)	0.014 (3)	0.006 (3)	0.013 (3)
C3	0.059 (4)	0.063 (4)	0.065 (4)	0.020 (3)	0.006 (3)	0.014 (3)
C4	0.057 (4)	0.070 (4)	0.069 (4)	0.023 (3)	0.006 (3)	0.002 (3)
C5	0.060 (4)	0.061 (4)	0.077 (4)	0.018 (3)	−0.002 (3)	−0.008 (3)
C6	0.052 (3)	0.049 (3)	0.078 (4)	0.014 (3)	0.001 (3)	0.005 (3)
C7	0.053 (3)	0.059 (4)	0.063 (4)	0.015 (3)	0.007 (3)	0.010 (3)
C8	0.051 (3)	0.049 (3)	0.062 (4)	0.012 (2)	0.000 (3)	0.011 (3)
C9	0.051 (3)	0.061 (3)	0.057 (3)	0.015 (3)	0.003 (3)	0.017 (3)
C10	0.052 (3)	0.063 (4)	0.068 (4)	0.011 (3)	0.004 (3)	0.014 (3)
C11	0.062 (4)	0.072 (4)	0.062 (4)	0.022 (3)	0.014 (3)	0.023 (3)
C12	0.062 (4)	0.064 (4)	0.058 (3)	0.026 (3)	0.003 (3)	0.015 (3)
C13	0.070 (4)	0.060 (4)	0.063 (4)	0.014 (3)	−0.006 (3)	0.007 (3)
C14	0.057 (4)	0.061 (4)	0.072 (4)	0.009 (3)	0.003 (3)	0.019 (3)
C15	0.083 (5)	0.095 (5)	0.073 (5)	0.027 (4)	0.008 (4)	0.008 (4)
C16	0.082 (5)	0.058 (4)	0.103 (6)	−0.001 (4)	0.005 (4)	0.012 (4)
C17	0.077 (5)	0.069 (4)	0.125 (7)	0.005 (4)	0.020 (5)	0.029 (4)

Geometric parameters (Å, °)

Br—C12	1.891 (6)	C9—C14	1.379 (8)
Br—O2^{i}	3.209 (6)	C9—C10	1.399 (8)
S—O2	1.464 (5)	C10—C11	1.374 (8)
S—C1	1.762 (6)	C10—H10	0.9300
S—C17	1.788 (8)	C11—C12	1.384 (9)
O1—C8	1.368 (7)	C11—H11	0.9300
O1—C7	1.375 (7)	C12—C13	1.371 (9)
C1—C8	1.371 (8)	C13—C14	1.392 (9)
C1—C2	1.456 (8)	C13—H13	0.9300
C2—C7	1.378 (8)	C14—H14	0.9300
C2—C3	1.396 (8)	C15—H15A	0.9600
C3—C4	1.372 (9)	C15—H15B	0.9600

C3—H3	0.9300	C15—H15C	0.9600
C4—C5	1.400 (10)	C16—H16A	0.9600
C4—C15	1.509 (10)	C16—H16B	0.9600
C5—C6	1.385 (9)	C16—H16C	0.9600
C5—H5	0.9300	C17—H17A	0.9600
C6—C7	1.380 (8)	C17—H17B	0.9600
C6—C16	1.505 (9)	C17—H17C	0.9600
C8—C9	1.470 (8)		
C12—Br—O2^{i}	165.1 (2)	C11—C10—H10	119.8
O2—S—C1	106.6 (3)	C9—C10—H10	119.8
O2—S—C17	106.1 (4)	C10—C11—C12	120.0 (6)
C1—S—C17	98.6 (3)	C10—C11—H11	120.0
C8—O1—C7	107.1 (4)	C12—C11—H11	120.0
C8—C1—C2	106.9 (5)	C13—C12—C11	120.5 (6)
C8—C1—S	125.5 (4)	C13—C12—Br	119.8 (5)
C2—C1—S	126.8 (4)	C11—C12—Br	119.5 (5)
C7—C2—C3	119.3 (6)	C12—C13—C14	119.3 (6)
C7—C2—C1	104.7 (5)	C12—C13—H13	120.3
C3—C2—C1	135.9 (5)	C14—C13—H13	120.3
C4—C3—C2	118.2 (6)	C9—C14—C13	121.1 (6)
C4—C3—H3	120.9	C9—C14—H14	119.4
C2—C3—H3	120.9	C13—C14—H14	119.4
C3—C4—C5	120.0 (6)	C4—C15—H15A	109.5
C3—C4—C15	120.3 (7)	C4—C15—H15B	109.5
C5—C4—C15	119.7 (6)	H15A—C15—H15B	109.5
C6—C5—C4	123.8 (6)	C4—C15—H15C	109.5
C6—C5—H5	118.1	H15A—C15—H15C	109.5
C4—C5—H5	118.1	H15B—C15—H15C	109.5
C7—C6—C5	113.5 (6)	C6—C16—H16A	109.5
C7—C6—C16	122.2 (6)	C6—C16—H16B	109.5
C5—C6—C16	124.2 (6)	H16A—C16—H16B	109.5
O1—C7—C2	111.1 (5)	C6—C16—H16C	109.5
O1—C7—C6	123.7 (5)	H16A—C16—H16C	109.5
C2—C7—C6	125.2 (6)	H16B—C16—H16C	109.5
O1—C8—C1	110.2 (5)	S—C17—H17A	109.5
O1—C8—C9	115.2 (5)	S—C17—H17B	109.5
C1—C8—C9	134.6 (5)	H17A—C17—H17B	109.5
C14—C9—C10	118.5 (6)	S—C17—H17C	109.5
C14—C9—C8	122.5 (5)	H17A—C17—H17C	109.5
C10—C9—C8	119.0 (5)	H17B—C17—H17C	109.5
C11—C10—C9	120.5 (6)		
O2—S—C1—C8	−124.5 (6)	C16—C6—C7—O1	1.6 (10)
C17—S—C1—C8	125.7 (6)	C5—C6—C7—C2	0.3 (9)
O2—S—C1—C2	44.1 (6)	C16—C6—C7—C2	−177.5 (6)
C17—S—C1—C2	−65.7 (6)	C7—O1—C8—C1	0.5 (6)
C8—C1—C2—C7	2.2 (6)	C7—O1—C8—C9	179.5 (5)
S—C1—C2—C7	−168.1 (5)	C2—C1—C8—O1	−1.7 (6)
C8—C1—C2—C3	178.5 (7)	S—C1—C8—O1	168.8 (4)

S—C1—C2—C3	8.1 (10)	C2—C1—C8—C9	179.6 (6)
C7—C2—C3—C4	−1.3 (9)	S—C1—C8—C9	−9.9 (10)
C1—C2—C3—C4	−177.1 (6)	O1—C8—C9—C14	159.4 (5)
C2—C3—C4—C5	1.9 (9)	C1—C8—C9—C14	−21.9 (10)
C2—C3—C4—C15	−179.4 (6)	O1—C8—C9—C10	−19.5 (8)
C3—C4—C5—C6	−1.5 (10)	C1—C8—C9—C10	159.2 (7)
C15—C4—C5—C6	179.8 (6)	C14—C9—C10—C11	0.3 (9)
C4—C5—C6—C7	0.3 (9)	C8—C9—C10—C11	179.2 (6)
C4—C5—C6—C16	178.1 (6)	C9—C10—C11—C12	1.0 (9)
C8—O1—C7—C2	1.0 (6)	C10—C11—C12—C13	−1.4 (9)
C8—O1—C7—C6	−178.2 (6)	C10—C11—C12—Br	−177.3 (5)
C3—C2—C7—O1	−179.0 (5)	C11—C12—C13—C14	0.5 (9)
C1—C2—C7—O1	−2.0 (6)	Br—C12—C13—C14	176.4 (5)
C3—C2—C7—C6	0.1 (9)	C10—C9—C14—C13	−1.2 (9)
C1—C2—C7—C6	177.2 (6)	C8—C9—C14—C13	179.9 (6)
C5—C6—C7—O1	179.4 (5)	C12—C13—C14—C9	0.8 (10)

Symmetry codes: (i) *x*, *y*, *z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16A···O2^{ii}	0.96	2.43	3.340 (10)	159

Symmetry codes: (ii) *x*, *y*−1, *z*.

Fig. 1

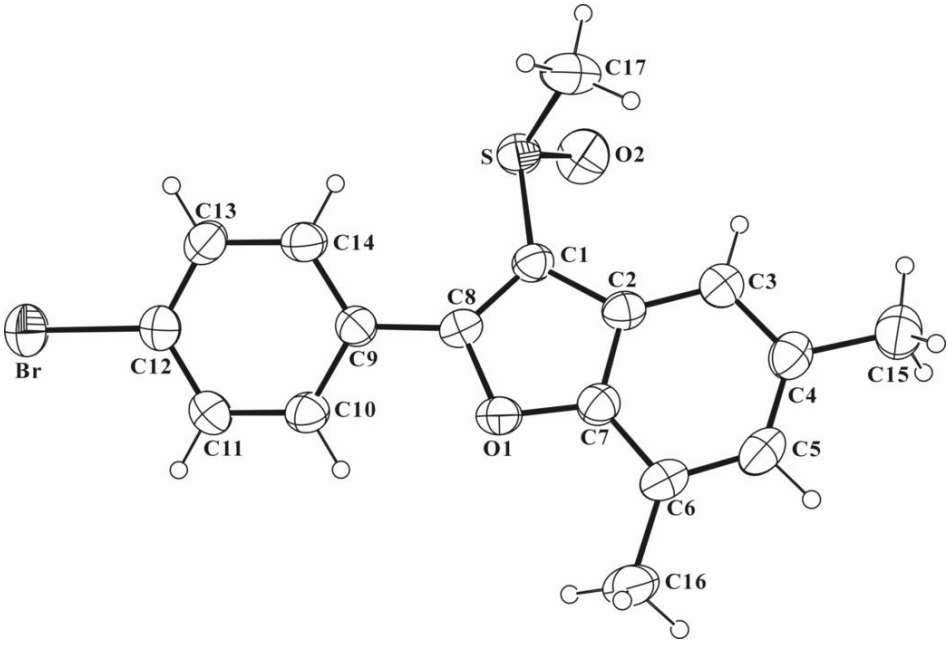

Fig. 2