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3-Bromomethyl-1-phenylsulfonyl-1*H*-indole-2-carbonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.006 Å
R factor = 0.044
wR factor = 0.120
Data-to-parameter ratio = 15.9

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

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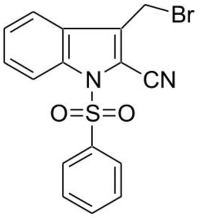
In the title molecule, $C_{16}H_{11}BrN_2O_2S$, the phenyl ring and mean plane of the indole ring system make a dihedral angle of 82.9 (1)°. Intermolecular C—H···O hydrogen bonds link the molecules into linear chains extended along the *a* axis. The crystal packing is further stabilized by van der Waals forces.

Comment

The indole ring system is present in a number of natural products and halogenated indole derivatives exhibit marked antibacterial activity against Gram-positive and Gram-negative bacteria and against fungi (Piscopo *et al.*, 1990). Some of the indole alkaloids extracted from plants possess interesting cytotoxic, antitumor or antiparasitic properties (Mukhopadhyay *et al.*, 1981). Sulfur-containing compounds act as simple diuretics (Crawford & Kennedy, 1959). In view of this biological importance and as a part of our studies on pharmacologically active indole derivatives, the crystal structure of the title compound, (I), was determined in order to establish the conformation of the molecule.



(I)

The bond lengths and angles (Table 1) are comparable to those observed in other phenylsulfonylindoles (Ravishankar *et al.*, 2005*a*,*b*). As a result of the electron-withdrawing character of the phenylsulfonyl group, the N—C*sp*^{2} bond lengths N1—C2 and N1—C5 (Table 1) are longer than the mean value of 1.355 (14) Å reported for N atoms with planar configurations (Allen *et al.*, 1987). Atom S1 has a distorted tetrahedral environment, with the O1—S1—O2 and N1—S1—C10 angles deviating significantly from ideal values, which may be attributed to the Thorpe–Ingold effect (Bassindale, 1984). The essential linearity of the carbonitrile group is evidenced from the bond angle C2—C16—N17. The orientation of the phenylsulfonyl group with respect to the planar indole ring system is influenced by the intramolecular C—H···O interaction involving sulfonyl atom O1 (Table 2). The phenyl ring and mean plane of the indole ring system make a dihedral angle of 82.9 (1)°.

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 2) link the molecules into linear chains extended

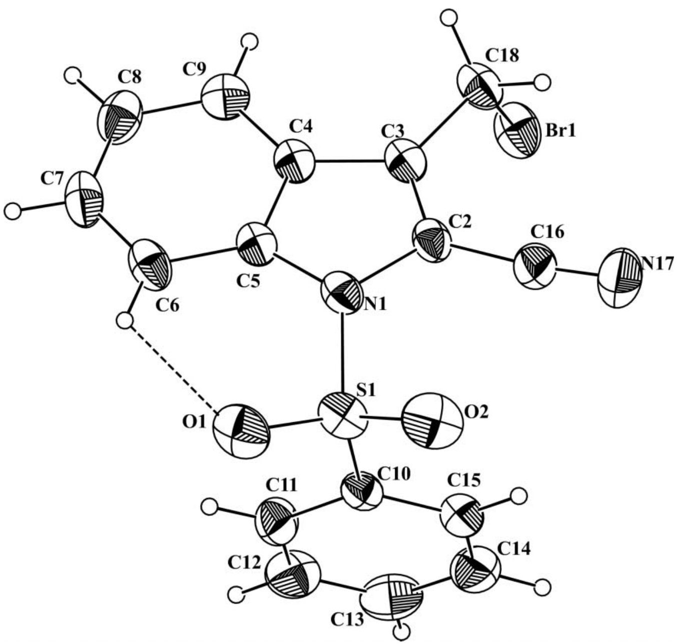


Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids. The dashed line indicates the intramolecular hydrogen bond.

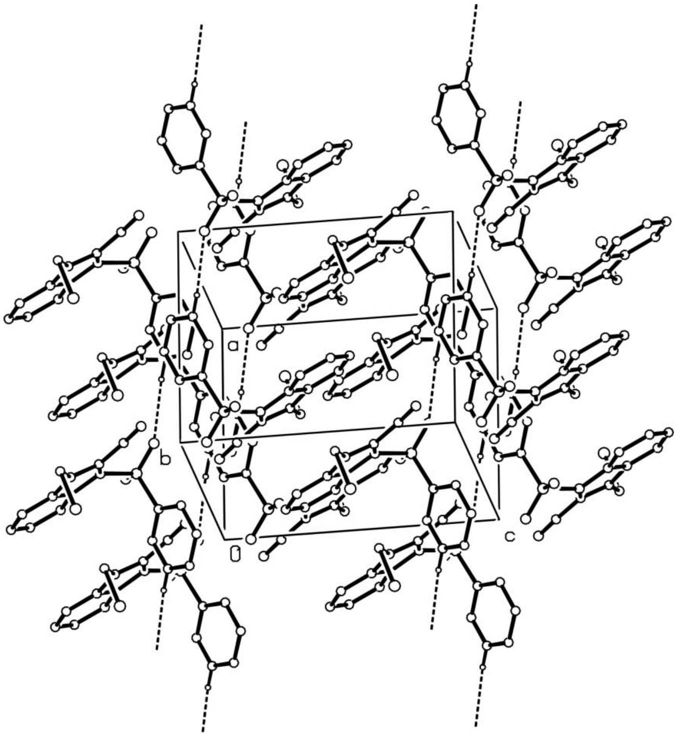


Figure 2
The molecular packing of (I). H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

along the *a* axis. The crystal packing (Fig. 2) is further stabilized by van der Waals forces.

Experimental

To a solution of 1-phenylsulfonyl-2-cyano-3-methylindole (10 mmol) in carbon tetrachloride (100 ml) finely powdered *N*-bromosuccinimide (2.13 g, 10.2 mmol) and dibenzoyl peroxide (20 mg) were added and the solution was refluxed for 4 h. The mixture was cooled to room temperature and the succinimide was filtered off. The filtrate was concentrated *in vacuo* to give 3-bromomethyl-2-carbonitrile-1-(phenylsulfonyl)indole as yellow crystals (yield 94%, m.p. 417 K). IR (KBr): 2213, 1372, 1179 cm^{-1}; ^{1}H NMR (400 MHz, CDCl$_3$): δ 4.66 (*s*, 2H, CH$_2$), 7.25–8.04 (*m*, 8H, Ar—H), 8.21–8.23 (*d*, 1H, *J* = 8.0 Hz, indole-7H); ^{13}C NMR (125 MHz, CDCl$_3$): δ 19.80, 107.55, 110.94, 114.87, 121.10, 126.51, 127.29, 129.42, 129.87, 132.56, 135.06, 136.80, 137.31.

Crystal data

$C_{16}H_{11}BrN_2O_2S$
$M_r = 375.24$
Triclinic, $P\overline{1}$
$a = 8.2689$ (14) Å
$b = 8.9841$ (15) Å
$c = 11.805$ (2) Å
$\alpha = 77.722$ (3)°
$\beta = 86.703$ (3)°
$\gamma = 64.795$ (3)°
$V = 774.8$ (2) Å^3
$Z = 2$
$D_x = 1.608$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6233 reflections
$\theta = 1.5$–27.4°
$\mu = 2.80$ mm^{-1}
$T = 293$ (2) K
Block, yellow
0.29 × 0.21 × 0.16 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.499$, $T_{\max} = 0.639$
6233 measured reflections
3157 independent reflections
2493 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.014$
$\theta_{\max} = 27.4°$
$h = -9 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -15 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.120$
$S = 1.03$
3157 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2 + 0.1871P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.67$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C18	1.959 (3)	S1—C10	1.744 (3)
S1—O2	1.417 (3)	N1—C2	1.405 (4)
S1—O1	1.420 (3)	N1—C5	1.406 (4)
S1—N1	1.690 (3)		
O2—S1—O1	121.29 (19)	C6—C5—C4	121.3 (3)
N1—S1—C10	103.37 (13)	N17—C16—C2	172.9 (5)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1	0.93	2.37	2.949 (5)	120
C12—H12···O2^{i}	0.93	2.53	3.385 (6)	153

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

H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 or 0.97 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C).

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:

Acta Cryst. (2006). E**62**, o440–o442 Palani *et al.* • $C_{16}H_{11}BrN_2O_2S$ **o441**

ZORTEP (Zsolnai, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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o442 Palani *et al.* • $C_{16}H_{11}BrN_2O_2S$ *Acta Cryst.* (2006). E**62**, o440–o442