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4-Bromo-*N*-(2-phenyl-1*H*-indol-7-yl)-benzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.043
wR factor = 0.108
Data-to-parameter ratio = 15.0

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

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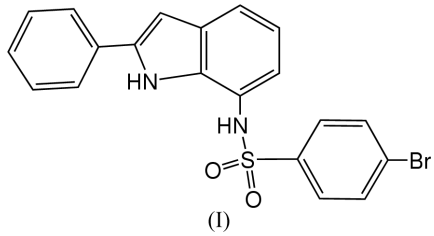
The title compound, $C_{20}H_{15}BrN_2O_2S$, is a new bioactive indole derivative with the 4-bromobenzenesulfonate moiety as a good leaving group. The S atom of the 4-bromobenzenesulfonate moiety is bonded to the amine N atom in sp^3 hybridization, with an S—N bond length of 1.616 (3) Å. The molecules are connected by N—H···O hydrogen bonds, forming one-dimensional columns along the *b* axis.

Comment

The title compound, (I), has a 4-bromobenzenesulfonate group bonded to the amine group in the indole moiety. Removal of the benzenesulfonate protecting group may further functionalize the indole derivative to produce a bioactive inhibitor. Thus, such indole derivatives with an amine group may be effective intermediates for the design of high-affinity antipsychotic drugs (Li *et al.*, 1999). There are only a few structural reports for these compounds to date (Sonar *et al.*, 2004). We have carried out an X-ray structural study of (I) in order to identify the hydrogen-bonding patterns created by the different NH groups.



(I)

The molecular structure of (I) is shown in Fig. 1, and important bond lengths and angles are given in Table 1. The C15–C20 phenyl ring makes a dihedral angle of 34.9 (2)° with the mean plane of the indole group (N2/C7–C14), in which the

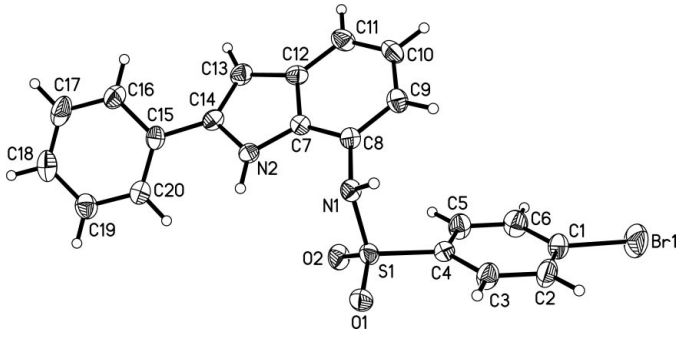


Figure 1
The molecular structure of (I), showing the atom-numbering scheme, and with displacement ellipsoids at the 50% probability level for non-H atoms.

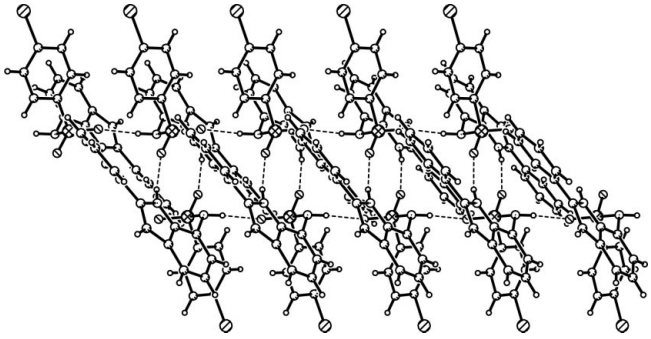


Figure 2
A packing diagram for (I), viewed down the *b* axis, showing the extended columns in the *b* direction. Dashed lines denote N—H···O hydrogen bonds.

atoms with the greatest deviations are N2 [−0.044 (4) Å] and C14 [0.046 (4) Å]. In the five-membered ring containing atom N2, the intra-ring bond angles range from 105.4 (3) to 109.0 (3)°; the N2—C7 and N2—C14 bond lengths are 1.371 (4) and 1.380 (4) Å, respectively, which indicates that the geometry around N2 is normal for sp^2 hybridization, as expected for π-conjugation of the indole ring.

The N1—C8 and N1—S1 bond lengths are 1.442 (4) and 1.616 (3) Å, respectively, indicative of standard single bonds, due to the sp^3-hybridized amine atom N1. The geometry around atom S1 is highly distorted tetrahedral, indicated by the O1—S1—O2 bond angle of 120.50 (14)°. The average S═O bond length is 1.418 (2) Å.

In the crystal structure of (I), a pair of head-to-tail intermolecular N2—H2*B*···O1($\frac{1}{2}-x$, $\frac{1}{2}-y$, $1-z$) hydrogen bonds (Table 2) link adjacent molecules to form a dimer. Each dimeric unit acts as a two-connected node, linking two adjacent dimer units *via* relatively strong N1—H1···O2(x, $y-1$, z) hydrogen bonds to form one-dimensional columns along the *b* axis (Fig. 2). There is no evidence of any aromatic π–π stacking of the indole rings.

Experimental

In the course of the synthesis of the pharmacologically active indole nucleus, the basic indole group was prepared from 2-amino-3-nitrophenol and phenylacetylene, according to the Sonogashira coupling reaction (Rodriguez *et al.*, 2000). The resulting 7-nitro-2-phenylindole was reduced to 7-amino-2-phenylindole with hydrogen over Pd/C and then converted to 4-bromo-*N*-(2-phenyl-1*H*-indol-7-yl)benzenesulfonamide, (I), using 4-bromobenzenesulfonyl chloride in pyridine and tetrahydrofuran (Park *et al.*, 1998). Colourless crystals of (I) were obtained by slow evaporation of an ethyl acetate solution.

Crystal data

$C_{20}H_{15}BrN_2O_2S$
M_r = 427.31
Monoclinic, $C2/c$
a = 30.764 (14) Å
b = 4.922 (2) Å
c = 26.335 (13) Å
β = 114.332 (8)°
V = 3633 (3) Å^3
Z = 8
D_x = 1.562 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2144 reflections
θ = 2.7–21.7°
μ = 2.40 mm^{-1}
T = 298 (2) K
Rod, colourless
0.40 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997*a*)
T_{min} = 0.607, T_{max} = 0.698
15 353 measured reflections
3524 independent reflections
2106 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 26.0°
$h = -37 \rightarrow 37$
$k = -6 \rightarrow 5$
$l = -32 \rightarrow 32$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.108
S = 0.96
3524 reflections
235 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C1	1.896 (3)	S1—C4	1.763 (3)
S1—O2	1.415 (2)	N1—C8	1.442 (4)
S1—O1	1.421 (2)	N2—C7	1.371 (4)
S1—N1	1.616 (3)	N2—C14	1.380 (4)
O2—S1—O1	120.50 (14)	O1—S1—C4	107.54 (14)
O2—S1—N1	107.16 (13)	N1—S1—C4	108.15 (13)
O1—S1—N1	106.13 (13)	C8—N1—S1	120.39 (19)
O2—S1—C4	106.88 (14)	C7—N2—C14	108.6 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.90	1.98	2.872 (3)	170
N2—H2*B*···O1^{ii}	0.90	2.13	3.009 (4)	167

Symmetry codes: (i) $x, y-1, z$; (ii) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$.

H atoms were placed in calculated positions (C—H = 0.95–0.99 Å and N—H = 0.88 Å and were allowed to ride on their parent atoms. The U_{iso}(H) values were set to 1.2U_{eq}(C) for the phenyl H atoms.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997*b*); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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