Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Bromomethyl-1-phenylsulfonyl-1*H*-indole

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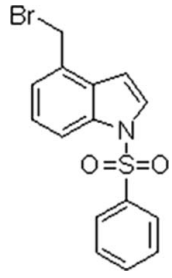
Received 12 March 2008; accepted 21 March 2008

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.008 Å; disorder in main residue; R factor = 0.062; wR factor = 0.199; data-to-parameter ratio = 18.9.

In the title molecule, $C_{15}H_{12}BrNO_2S$, the indole mean plane and phenyl ring are nearly orthogonal to each other, forming a dihedral angle of 88.19 (13)°. The Br atom is disordered over two close positions with occupancies of 0.56 (4) and 0.44 (4). The crystal packing exhibits weak intermolecular C—H$\cdots\pi$ interactions.

Related literature

For related crystal structures, see: Chakkaravarthi *et al.* (2007, 2008). For biological activities of indole derivatives, see: Okabe & Adachi (1998); Schollmeyer *et al.* (1995).



Experimental

Crystal data

$C_{15}H_{12}BrNO_2S$
M_r = 350.23
Monoclinic, $P2_1/c$
a = 11.7060 (9) Å
b = 8.2399 (7) Å
c = 15.4495 (11) Å
β = 103.858 (3)°
V = 1446.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.98 mm^{-1}
T = 295 (2) K
0.18 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEX2 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.566, T_{max} = 0.620
16472 measured reflections
3606 independent reflections
2160 reflections with $I > 2s(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.199
S = 1.06
3606 reflections
191 parameters
8 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C13—H13$\cdots Cg1^{i}$	0.93	2.83	3.716 (6)	160
C9—H9$D\cdots Cg1^{ii}$	0.97	2.92	3.673 (5)	135
C1—H1$\cdots Cg2^{iii}$	0.93	2.69	3.584 (6)	162

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$. $Cg1$ and $Cg2$ are the centroids of atoms C3–C8 and C10–C15, respectively.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2* program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge the Sophisticated Analytical Instrument Facility, Indian Institute of Technology, Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2392).

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supporting information

Acta Cryst. (2008). E**64**, o751 [doi:10.1107/S1600536808007794]

4-Bromomethyl-1-phenylsulfonyl-1*H*-indole

G. Chakkaravarthi, Radhakrishnan Sureshbabu, A. K. Mohanakrishnan and V. Manivannan

S1. Comment

The indole derivatives are found to possess antibacterial (Okabe and Adachi, 1998) and antitumour (Schollmeyer *et al.*, 1995) activities. In continuation of our studies in indole derivatives, we present the crystal structure of the title compound (I).

The geometric parameters of (I) (Fig. 1) agree with those in the reported structures (Chakkaravarthi *et al.*, 2007; 2008) The indole mean plane and phenyl ring are nearly orthogonal to each other forming a dihedral angle of 88.19 (13)°. The plane of N1/S1/C1 makes the dihedral angles of 84.30 (14)°) and 72.38 (16)°, respectively, with the indole mean plane and phenyl ring. The sum of bond angles around N1 (356.9°) indicates that N1 is sp^2-hybridized. The torsion angles C11-C10-S1-O2 [-6.3 (5)°] and C15-C10-S1-O1 [39.4 (5)°] indicate the *syn* conformation of the sulfonyl moiety.

The crystal packing exhibits weak intermolecular C—H···π interactions, involving the rings C3-C8 (centroid *Cg*1) and C10-C15 (centroid *Cg*2) (Table 1).

S2. Experimental

4-(Methyl)-1-(phenylsulfonyl)-1*H*-indole (1 g, 2.8 m.mol), *N*-bromo succinimide (0.5 g, 3 m.mol), azobis isobutyro nitrile (50 mg) were dissolved in 50 ml of carbon tetra chloride and refluxed on a waterbath for 2 h, then cooled to the room temperature. Succinimide was filtered off over sodium sulfate. Filtrate was evaporated under reduced pressure. Product was recrystallized from methanol. Yield: 80 %.

S3. Refinement

H atoms were positioned geometrically and refined using riding model with C-H = 0.93-0.97 Å, and U_{iso}(H) = 1.2Ueq(C). The Br atom was treated as disordered over two close positions with the occupancies of 0.56 (4) and 0.44 (4), respectively. The distances C4-C5, C10-C11, C11-C12, C12-C13, C13-C14, C14-C15, C15-C10 were restrained to 1.395 (5) Å and the distance C9-Br1A was restrained to 1.91 (10) Å. The positive residual peak 1.26 e Å^{-3} is located at 1.62 Å from C9; the peak might be the disordered component of Br with small occupancy. It was ignored as showing no any structural or packing consequences.

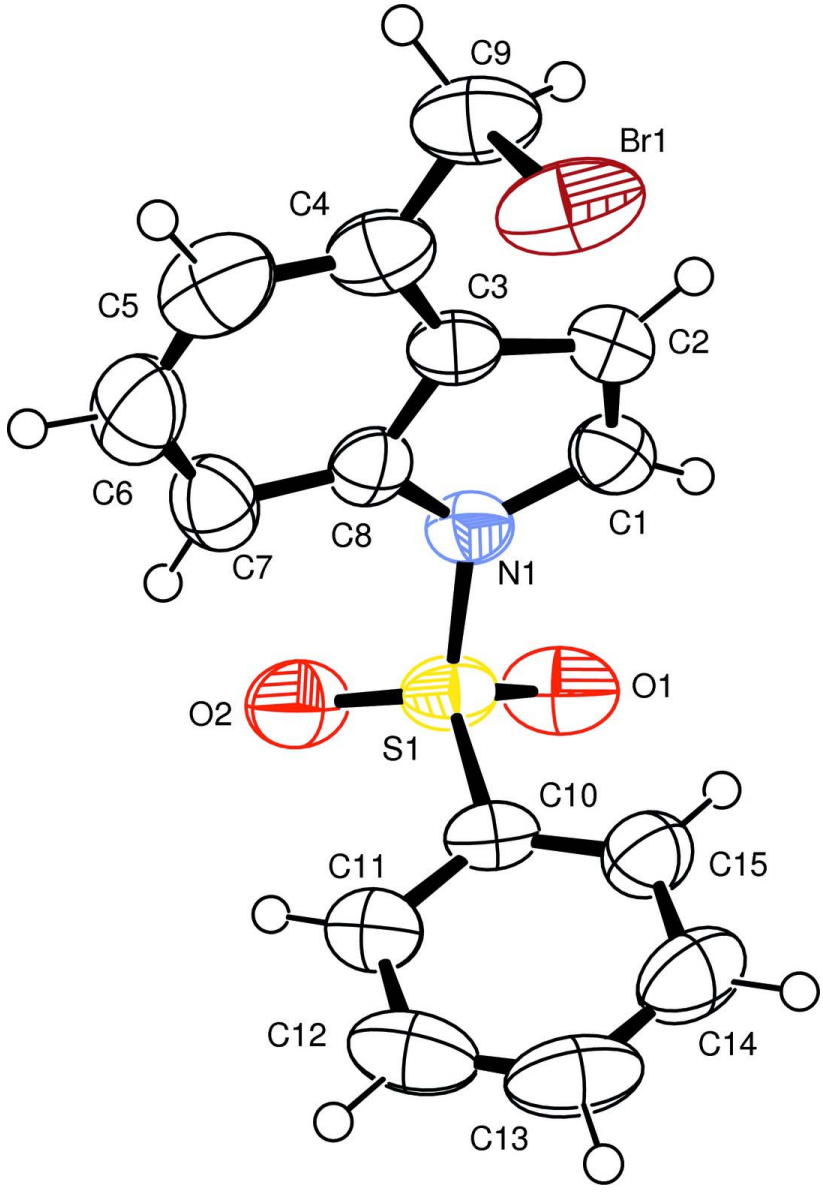

Figure 1

The molecular structure of (I) showing the atomic labels and 50% probability displacement ellipsoids for non-H atoms. Only major parts of the disordered atoms are drawn.

4-Bromomethyl-1-phenylsulfonyl-1*H*-indole

Crystal data

$C_{15}H_{12}BrNO_2S$
$M_r = 350.23$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.7060\ (9)$ Å
$b = 8.2399\ (7)$ Å
$c = 15.4495\ (11)$ Å
$\beta = 103.858\ (3)°$
$V = 1446.8\ (2)$ Å^3
$Z = 4$
$F(000) = 704$
$D_x = 1.608$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5113 reflections
$\theta = 2.5–25.8°$
$\mu = 2.99$ mm^{-1}

T = 295 K
Block, colourless

0.18 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEX2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.566, T_{max} = 0.620

16472 measured reflections
3606 independent reflections
2160 reflections with $I > 2s(I)$
R_{int} = 0.041
θ_{max} = 28.6°, θ_{min} = 1.8°
h = −15→15
k = −10→11
l = −12→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.199
S = 1.06
3606 reflections
191 parameters
8 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.089P)^2 + 1.9138P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.7826 (5)	0.6808 (6)	0.2167 (3)	0.0595 (13)	
H1	0.8345	0.7022	0.1810	0.071*	
C2	0.7274 (4)	0.7938 (6)	0.2531 (3)	0.0576 (12)	
H2	0.7326	0.9055	0.2463	0.069*	
C3	0.6578 (4)	0.7104 (6)	0.3052 (3)	0.0501 (11)	
C4	0.5821 (4)	0.7671 (7)	0.3555 (3)	0.0605 (13)	
C5	0.5258 (5)	0.6520 (8)	0.3953 (4)	0.0771 (18)	
H5	0.4734	0.6856	0.4284	0.092*	
C6	0.5457 (6)	0.4882 (9)	0.3870 (4)	0.0769 (18)	
H6	0.5063	0.4147	0.4151	0.092*	
C7	0.6223 (5)	0.4290 (7)	0.3385 (4)	0.0643 (14)	
H7	0.6367	0.3186	0.3345	0.077*	
C8	0.6757 (4)	0.5440 (6)	0.2967 (3)	0.0489 (11)	
C10	0.9404 (4)	0.3588 (5)	0.3317 (3)	0.0502 (11)	
C11	0.9363 (5)	0.2442 (6)	0.3965 (3)	0.0673 (14)	
H11	0.8754	0.1690	0.3884	0.081*	
C12	1.0253 (5)	0.2450 (8)	0.4736 (3)	0.0833 (19)	
H12	1.0248	0.1697	0.5183	0.100*	
C13	1.1153 (5)	0.3580 (7)	0.4842 (4)	0.0805 (19)	
H13	1.1751	0.3569	0.5361	0.097*	
C14	1.1177 (5)	0.4719 (7)	0.4194 (3)	0.0765 (17)	
H14	1.1783	0.5477	0.4277	0.092*	
C15	1.0293 (4)	0.4726 (6)	0.3419 (3)	0.0621 (13)	

H15	1.0297	0.5484	0.2973	0.075*	
N1	0.7516 (3)	0.5255 (5)	0.2396 (3)	0.0524 (10)	
O1	0.8833 (4)	0.3941 (6)	0.1596 (2)	0.0771 (12)	
O2	0.7575 (3)	0.2269 (5)	0.2295 (3)	0.0775 (11)	
S1	0.83141 (11)	0.36176 (16)	0.23203 (8)	0.0569 (4)	
C9	0.5669 (4)	0.9457 (7)	0.3700 (3)	0.0725 (16)	
H9A	0.4865	0.9665	0.3734	0.087*	0.56 (4)
H9B	0.5813	1.0060	0.3198	0.087*	0.56 (4)
H9C	0.4898	0.9633	0.3813	0.087*	0.44 (4)
H9D	0.5701	1.0035	0.3160	0.087*	0.44 (4)
Br1	0.6721 (4)	1.0180 (7)	0.4768 (3)	0.0792 (10)	0.56 (4)
Br1A	0.6841 (7)	1.0268 (5)	0.4688 (5)	0.0844 (16)	0.44 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.057 (3)	0.061 (3)	0.062 (3)	0.007 (3)	0.017 (2)	0.013 (2)
C2	0.055 (3)	0.051 (3)	0.066 (3)	0.006 (2)	0.012 (2)	0.010 (2)
C3	0.047 (2)	0.059 (3)	0.038 (2)	0.008 (2)	−0.0024 (18)	0.0035 (19)
C4	0.054 (3)	0.081 (4)	0.040 (2)	0.013 (3)	−0.001 (2)	0.002 (2)
C5	0.067 (4)	0.115 (6)	0.052 (3)	0.014 (4)	0.020 (3)	0.005 (3)
C6	0.071 (4)	0.103 (5)	0.059 (3)	−0.008 (3)	0.019 (3)	0.020 (3)
C7	0.069 (3)	0.062 (3)	0.056 (3)	−0.009 (3)	0.005 (3)	0.008 (2)
C8	0.040 (2)	0.063 (3)	0.037 (2)	−0.002 (2)	−0.0032 (17)	0.0036 (19)
C10	0.047 (2)	0.054 (3)	0.046 (2)	0.014 (2)	0.0038 (19)	−0.005 (2)
C11	0.063 (3)	0.065 (3)	0.071 (3)	0.008 (3)	0.009 (3)	0.008 (3)
C12	0.100 (5)	0.087 (4)	0.057 (3)	0.035 (4)	0.007 (3)	0.015 (3)
C13	0.072 (4)	0.093 (5)	0.061 (3)	0.030 (4)	−0.017 (3)	−0.022 (3)
C14	0.052 (3)	0.088 (4)	0.079 (4)	−0.002 (3)	−0.006 (3)	−0.019 (3)
C15	0.054 (3)	0.064 (3)	0.065 (3)	0.000 (3)	0.007 (2)	−0.002 (2)
N1	0.049 (2)	0.057 (2)	0.049 (2)	0.0085 (18)	0.0068 (17)	0.0049 (17)
O1	0.090 (3)	0.096 (3)	0.0455 (19)	0.027 (2)	0.0168 (18)	−0.0023 (19)
O2	0.068 (2)	0.062 (2)	0.090 (3)	0.001 (2)	−0.005 (2)	−0.014 (2)
S1	0.0549 (7)	0.0595 (8)	0.0494 (7)	0.0101 (6)	−0.0010 (5)	−0.0080 (5)
C9	0.074 (4)	0.090 (4)	0.050 (3)	0.030 (3)	0.006 (3)	0.002 (3)
Br1	0.0703 (18)	0.118 (3)	0.0437 (13)	0.035 (2)	0.0030 (8)	−0.0089 (11)
Br1A	0.120 (4)	0.059 (2)	0.068 (2)	−0.016 (3)	0.0095 (16)	0.0012 (13)

Geometric parameters (Å, º)

C1—C2	1.332 (7)	C11—C12	1.381 (4)
C1—N1	1.398 (7)	C11—H11	0.9300
C1—H1	0.9300	C12—C13	1.386 (5)
C2—C3	1.448 (7)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.379 (4)
C3—C4	1.392 (7)	C13—H13	0.9300
C3—C8	1.398 (7)	C14—C15	1.382 (4)
C4—C5	1.380 (4)	C14—H14	0.9300

C4—C9	1.505 (8)	C15—H15	0.9300
C5—C6	1.381 (9)	N1—S1	1.661 (4)
C5—H5	0.9300	O1—S1	1.421 (4)
C6—C7	1.387 (9)	O2—S1	1.403 (4)
C6—H6	0.9300	C9—Br1	1.903 (6)
C7—C8	1.379 (7)	C9—Br1A	1.9115 (10)
C7—H7	0.9300	C9—H9A	0.9700
C8—N1	1.402 (6)	C9—H9B	0.9700
C10—C15	1.381 (4)	C9—H9C	0.9700
C10—C11	1.386 (4)	C9—H9D	0.9700
C10—S1	1.749 (4)		

C2—C1—N1	110.6 (4)	C12—C13—H13	119.4
C2—C1—H1	124.7	C13—C14—C15	119.4 (5)
N1—C1—H1	124.7	C13—C14—H14	120.3
C1—C2—C3	107.3 (5)	C15—C14—H14	120.3
C1—C2—H2	126.4	C10—C15—C14	118.9 (5)
C3—C2—H2	126.4	C10—C15—H15	120.5
C4—C3—C8	120.7 (5)	C14—C15—H15	120.5
C4—C3—C2	132.0 (5)	C1—N1—C8	107.5 (4)
C8—C3—C2	107.2 (4)	C1—N1—S1	122.8 (4)
C5—C4—C3	117.0 (5)	C8—N1—S1	125.8 (3)
C5—C4—C9	121.2 (5)	O2—S1—O1	120.3 (3)
C3—C4—C9	121.7 (5)	O2—S1—N1	107.0 (2)
C4—C5—C6	121.4 (6)	O1—S1—N1	104.9 (2)
C4—C5—H5	119.3	O2—S1—C10	109.2 (2)
C6—C5—H5	119.3	O1—S1—C10	109.7 (2)
C5—C6—C7	122.6 (6)	N1—S1—C10	104.7 (2)
C5—C6—H6	118.7	C4—C9—Br1	111.1 (4)
C7—C6—H6	118.7	C4—C9—Br1A	111.9 (3)
C8—C7—C6	115.8 (6)	C4—C9—H9A	109.4
C8—C7—H7	122.1	Br1—C9—H9A	109.4
C6—C7—H7	122.1	Br1A—C9—H9A	114.5
C7—C8—C3	122.4 (5)	C4—C9—H9B	109.4
C7—C8—N1	130.3 (5)	Br1—C9—H9B	109.4
C3—C8—N1	107.3 (4)	Br1A—C9—H9B	103.3
C15—C10—C11	122.4 (4)	H9A—C9—H9B	108.0
C15—C10—S1	117.5 (3)	C4—C9—H9C	108.8
C11—C10—S1	120.1 (3)	Br1—C9—H9C	103.5
C12—C11—C10	118.1 (5)	Br1A—C9—H9C	108.9
C12—C11—H11	121.0	H9B—C9—H9C	114.5
C10—C11—H11	121.0	C4—C9—H9D	108.7
C11—C12—C13	120.0 (5)	Br1—C9—H9D	116.2
C11—C12—H12	120.0	Br1A—C9—H9D	110.3
C13—C12—H12	120.0	H9A—C9—H9D	101.4
C14—C13—C12	121.2 (5)	H9C—C9—H9D	108.2
C14—C13—H13	119.4		

N1—C1—C2—C3	1.5 (6)	C13—C14—C15—C10	0.2 (9)
C1—C2—C3—C4	−178.7 (5)	C2—C1—N1—C8	−2.3 (6)
C1—C2—C3—C8	−0.2 (5)	C2—C1—N1—S1	−161.2 (4)
C8—C3—C4—C5	−0.4 (7)	C7—C8—N1—C1	−179.0 (5)
C2—C3—C4—C5	178.0 (5)	C3—C8—N1—C1	2.1 (5)
C8—C3—C4—C9	176.4 (4)	C7—C8—N1—S1	−20.9 (7)
C2—C3—C4—C9	−5.2 (7)	C3—C8—N1—S1	160.2 (3)
C3—C4—C5—C6	1.3 (8)	C1—N1—S1—O2	−159.9 (4)
C9—C4—C5—C6	−175.5 (5)	C8—N1—S1—O2	45.2 (4)
C4—C5—C6—C7	−0.2 (10)	C1—N1—S1—O1	−31.1 (5)
C5—C6—C7—C8	−1.6 (9)	C8—N1—S1—O1	174.0 (4)
C6—C7—C8—C3	2.5 (7)	C1—N1—S1—C10	84.4 (4)
C6—C7—C8—N1	−176.3 (5)	C8—N1—S1—C10	−70.6 (4)
C4—C3—C8—C7	−1.5 (7)	C15—C10—S1—O2	173.1 (4)
C2—C3—C8—C7	179.7 (4)	C11—C10—S1—O2	−6.3 (5)
C4—C3—C8—N1	177.5 (4)	C15—C10—S1—O1	39.4 (5)
C2—C3—C8—N1	−1.2 (5)	C11—C10—S1—O1	−140.0 (4)
C15—C10—C11—C12	−0.3 (8)	C15—C10—S1—N1	−72.7 (4)
S1—C10—C11—C12	179.0 (4)	C11—C10—S1—N1	108.0 (4)
C10—C11—C12—C13	−0.1 (9)	C5—C4—C9—Br1	84.3 (6)
C11—C12—C13—C14	0.6 (9)	C3—C4—C9—Br1	−92.4 (6)
C12—C13—C14—C15	−0.6 (9)	C5—C4—C9—Br1A	91.4 (7)
C11—C10—C15—C14	0.3 (8)	C3—C4—C9—Br1A	−85.3 (6)
S1—C10—C15—C14	−179.1 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···*Cg*1^{i}	0.93	2.83	3.716 (6)	160
C9—H9*D*···*Cg*1^{ii}	0.97	2.92	3.673 (5)	135
C1—H1···*Cg*2^{iii}	0.93	2.69	3.584 (6)	162

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, *y*+1/2, −*z*+1/2; (iii) −*x*+2, *y*+1/2, −*z*+1/2.