Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Bromophenyl)methanesulfonamide

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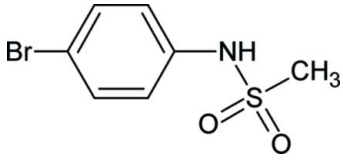
Received 6 April 2007; accepted 17 April 2007

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; R factor = 0.026; wR factor = 0.072; data-to-parameter ratio = 14.3.

The structure of the title compound, $C_7H_8BrNO_2S$, closely resembles those of other alkyl sulfonanilides. The molecules in the crystal structure are linked into zigzag chains in the *b*-axis direction *via* N—H···O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2000, 2007, 2007*a*,*b*,*c*,*d*,*e*,*f*); Jayalakshmi & Gowda (2004); Klug (1968).



Experimental

Crystal data

$C_7H_8BrNO_2S$
M_r = 250.11
Monoclinic, $P2_1/c$
a = 9.7474 (6) Å
b = 5.7660 (3) Å
c = 16.378 (1) Å
β = 97.272 (6)°
V = 913.10 (9) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 7.97 mm^{-1}
T = 299 (2) K
0.28 × 0.25 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.182, T_{max} = 0.344 (expected range = 0.160–0.303)
1972 measured reflections
1625 independent reflections
1508 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
3 standard reflections
frequency: 120 min
intensity decay: 4.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.072
S = 1.08
1625 reflections
114 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5*N*···O3^{i}	0.854 (10)	2.229 (16)	3.027 (3)	155 (3)

Symmetry code: (i) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CAD-4-PC* (Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

BTG gratefully thanks the Alexander von Humboldt Foundation, Bonn, Germany for an extension of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2338).

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 doi:10.1107/S1600536807019009

supplementary materials

Acta Cryst. (2007). E**63**, o2597 [**doi:10.1107/S1600536807019009**]

N-(4-Bromophenyl)methanesulfonamide

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Comment

The alkyl sulfonanilides are an important class of biologically significant compounds. The stereochemistry of these compounds particularly in the vicinity of the phenyl-N—H portion is of interest as it helps in explaining their biological activity. In the present work, the structure of N-(4-bromophenyl)-methanesulfonamde has been determined (Fig. 1) to explore the substituent effects on the structures of anilides and sulfonanilides (Gowda et al., 2007a-f; Gowda, Kozisek et al., 2007; Gowda, Paulus et al., 2000). Geometric parameters in these structures are similar. Like in other alkyl sulfonanilides (Gowda et al., 2007b-f), the amide hydrogen is available to a receptor molecule. The molecules in the title compound are packed zigzag chains in the direction of the b axis via N—H···O hydrogen bonds.

Experimental

The title compound was prepared according to the literature method (Jayalakshmi & Gowda, 2004). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Jayalakshmi & Gowda, 2004). Single crystals of the title compound were obtained from a slow evaporation of its ethanolic solution and used for X-ray diffraction studied at room temperature.

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (CH aromatic) or 0.96 Å (CH_3) and U_{iso}(H) = 1.2 U_{eq}(C,*N*) or U_{iso}(H) = 1.5 U_{eq}(C_{methyl}). The methyl group was allowed to rotate but not to tip. The coordinates of the H atom bonded to N were refined with distance restraint of 0.86 (1) Å.

Figures

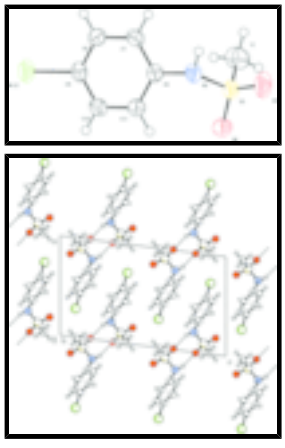

Fig. 1. The molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

N-(4-Bromophenyl)methanesulfonamide

Crystal data

$C_7H_8BrNO_2S$	F_{000} = 496
M_r = 250.11	D_x = 1.819 Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation λ = 1.54180 Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
a = 9.7474 (6) Å	θ = 9.2–25.4º
b = 5.7660 (3) Å	μ = 7.97 mm^{-1}
c = 16.3780 (10) Å	T = 299 (2) K
β = 97.272 (6)º	Prism, grey
V = 913.10 (9) Å^3	0.28 × 0.25 × 0.15 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.030
Radiation source: fine-focus sealed tube	θ_{max} = 67.0º
Monochromator: graphite	θ_{min} = 4.6º
T = 299(2) K	h = −11→11
ω/2θ scans	k = 0→6
Absorption correction: ψ scan (North *et al.*, 1968)	l = −19→3
T_{min} = 0.182, T_{max} = 0.344	3 standard reflections
1972 measured reflections	every 120 min
1625 independent reflections	intensity decay: 4.0%
1508 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.7498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.026	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.072	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
S = 1.08	$\Delta\rho_{min}$ = −0.50 e Å^{-3}
1625 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
114 parameters	Extinction coefficient: 0.0106 (4)
1 restraint	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Hydrogen site location: inferred from neighbouring sites

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
C1	0.9894 (4)	0.2605 (7)	0.1006 (2)	0.0638 (9)
H1A	1.0507	0.2175	0.0616	0.077*
H1B	1.0415	0.3335	0.1473	0.077*
H1C	0.9211	0.3667	0.0752	0.077*
C6	0.6817 (3)	0.2435 (5)	0.16508 (14)	0.0321 (5)
C7	0.6694 (3)	0.4593 (5)	0.20045 (15)	0.0377 (6)
H7	0.7407	0.5162	0.2382	0.045*
C8	0.5514 (3)	0.5904 (5)	0.17978 (16)	0.0381 (6)
H8	0.5415	0.7337	0.2045	0.046*
C9	0.4487 (3)	0.5057 (5)	0.12209 (15)	0.0353 (5)
C10	0.4604 (3)	0.2940 (5)	0.08516 (16)	0.0401 (6)
H10	0.3905	0.2408	0.0457	0.048*
C11	0.5773 (3)	0.1603 (5)	0.10720 (16)	0.0383 (6)
H11	0.5856	0.0156	0.0833	0.046*
Br12	0.28668 (3)	0.68488 (6)	0.093223 (19)	0.05147 (17)
N5	0.7988 (2)	0.1016 (4)	0.19397 (13)	0.0386 (5)
H5N	0.842 (3)	0.153 (5)	0.2390 (11)	0.046*
O3	1.0074 (2)	−0.1222 (5)	0.18364 (14)	0.0638 (6)
O4	0.8323 (2)	−0.0930 (4)	0.06242 (12)	0.0517 (5)
S2	0.90772 (6)	0.01280 (12)	0.13265 (4)	0.0390 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.062 (2)	0.073 (2)	0.059 (2)	−0.0159 (19)	0.0183 (16)	−0.0057 (18)
C6	0.0311 (12)	0.0384 (13)	0.0274 (11)	0.0015 (10)	0.0053 (9)	0.0013 (10)
C7	0.0338 (13)	0.0419 (14)	0.0358 (12)	−0.0028 (11)	−0.0014 (10)	−0.0026 (11)
C8	0.0402 (14)	0.0352 (13)	0.0385 (13)	0.0017 (11)	0.0040 (11)	−0.0026 (11)
C9	0.0312 (12)	0.0428 (14)	0.0321 (12)	0.0049 (11)	0.0047 (10)	0.0056 (10)
C10	0.0348 (13)	0.0487 (16)	0.0352 (13)	0.0005 (12)	−0.0017 (10)	−0.0038 (11)
C11	0.0369 (13)	0.0412 (15)	0.0359 (13)	0.0020 (11)	0.0007 (10)	−0.0063 (11)

Br12	0.0401 (2)	0.0586 (3)	0.0540 (2)	0.01533 (13)	−0.00079 (13)	0.00234 (14)
N5	0.0357 (12)	0.0502 (13)	0.0287 (10)	0.0085 (10)	−0.0003 (8)	−0.0006 (10)
O3	0.0501 (13)	0.0814 (16)	0.0569 (13)	0.0321 (12)	−0.0044 (10)	0.0007 (12)
O4	0.0473 (11)	0.0620 (13)	0.0441 (11)	0.0060 (10)	−0.0006 (9)	−0.0187 (10)
S2	0.0326 (3)	0.0485 (4)	0.0350 (3)	0.0082 (3)	0.0002 (2)	−0.0043 (3)

Geometric parameters (Å, °)

C1—S2	1.748 (4)	C8—H8	0.9300
C1—H1A	0.9600	C9—C10	1.374 (4)
C1—H1B	0.9600	C9—Br12	1.897 (2)
C1—H1C	0.9600	C10—C11	1.384 (4)
C6—C7	1.384 (4)	C10—H10	0.9300
C6—C11	1.386 (4)	C11—H11	0.9300
C6—N5	1.435 (3)	N5—S2	1.634 (2)
C7—C8	1.382 (4)	N5—H5N	0.854 (10)
C7—H7	0.9300	O3—S2	1.429 (2)
C8—C9	1.376 (4)	O4—S2	1.422 (2)
S2—C1—H1A	109.5	C8—C9—Br12	119.2 (2)
S2—C1—H1B	109.5	C9—C10—C11	119.4 (2)
H1A—C1—H1B	109.5	C9—C10—H10	120.3
S2—C1—H1C	109.5	C11—C10—H10	120.3
H1A—C1—H1C	109.5	C10—C11—C6	119.6 (2)
H1B—C1—H1C	109.5	C10—C11—H11	120.2
C7—C6—C11	120.1 (2)	C6—C11—H11	120.2
C7—C6—N5	118.8 (2)	C6—N5—S2	121.86 (16)
C11—C6—N5	120.9 (2)	C6—N5—H5N	112 (2)
C8—C7—C6	120.2 (2)	S2—N5—H5N	111 (2)
C8—C7—H7	119.9	O4—S2—O3	118.86 (15)
C6—C7—H7	119.9	O4—S2—N5	108.81 (12)
C9—C8—C7	119.0 (2)	O3—S2—N5	104.97 (12)
C9—C8—H8	120.5	O4—S2—C1	108.44 (16)
C7—C8—H8	120.5	O3—S2—C1	108.57 (19)
C10—C9—C8	121.6 (2)	N5—S2—C1	106.54 (16)
C10—C9—Br12	119.18 (19)		
C11—C6—C7—C8	1.6 (4)	C7—C6—C11—C10	−0.2 (4)
N5—C6—C7—C8	−173.7 (2)	N5—C6—C11—C10	175.0 (2)
C6—C7—C8—C9	−1.7 (4)	C7—C6—N5—S2	−120.9 (2)
C7—C8—C9—C10	0.4 (4)	C11—C6—N5—S2	63.8 (3)
C7—C8—C9—Br12	−179.9 (2)	C6—N5—S2—O4	−51.5 (3)
C8—C9—C10—C11	1.0 (4)	C6—N5—S2—O3	−179.7 (2)
Br12—C9—C10—C11	−178.7 (2)	C6—N5—S2—C1	65.2 (3)
C9—C10—C11—C6	−1.1 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···O3^{i}	0.854 (10)	2.229 (16)	3.027 (3)	155 (3)

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

Fig. 1

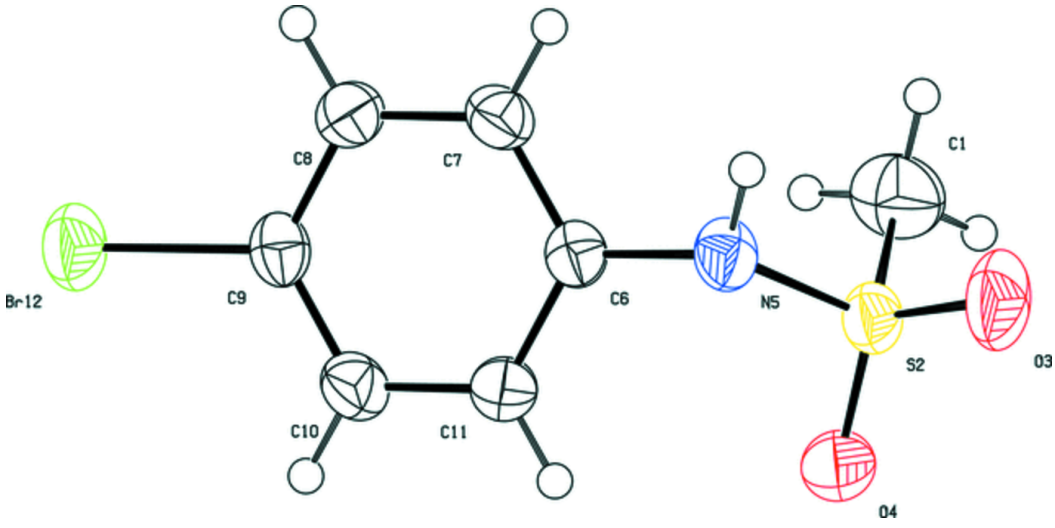

Fig. 2