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N-(4-Aminobenzyl)-*N*,4-dimethylbenzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.047
wR factor = 0.132
Data-to-parameter ratio = 15.8

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

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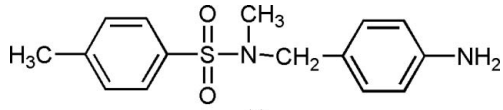
In the title compound, $C_{15}H_{18}N_2O_2S$, the angle between the two benzene rings is 96.3 (3) Å. In the crystal structure, molecules are linked *via* intermolecular N—H···O and C—H···O interactions.

Comment

Sulfonamides (*R1*SO_2–N*H*R2) are a common pharmacophore in various biologically active molecules, enzyme inhibitors and receptor antagonists (Lendnicer & Mitscher, 1977; Raju *et al.*, 1996; Raju & Timothy, 1997). This paper reports the structure of *N*-(4-aminobenzyl)-*N*,4-dimethylbenzenesulfonamide, (I) (Fig. 1) (Andemen *et al.*, 1988), in which the angle between two benzene rings (C1–C6 and C9–C14) is 96.3 (3)°.



(I)

In the crystal structure, N—H···O hydrogen bonds link adjacent molecules into inversion-related dimers. The structure is further stabilized by weak C—H···O hydrogen bonds (Fig. 2 and Table 1).

Experimental

The title compound, (I), was synthesized according to the procedure of Andemen *et al.* (1988). Crystals suitable for X-ray analysis were grown by slow evaporation of an absolute ethanol solution at room temperature over a period of 15 d.

Crystal data

$C_{15}H_{18}N_2O_2S$
M_r = 290.37
Monoclinic, $P2_1/c$
a = 15.939 (5) Å
b = 8.012 (2) Å
c = 11.997 (3) Å
β = 105.919 (5)°
V = 1473.3 (7) Å^3
Z = 4
D_x = 1.309 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 294 (2) K
Block, colourless
0.34 × 0.24 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.912, T_{max} = 0.974
7932 measured reflections
2991 independent reflections
1342 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.132$
$S = 0.94$
2991 reflections
189 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.870 (16)	2.57 (2)	3.347 (4)	148 (3)
C5—H5···O1^{ii}	0.93	2.57	3.498 (4)	173

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $x, y-1, z$.

The H atoms bound to N2 were found in a difference Fourier map and refined with U_{iso}(H) = 1.2U_{eq}(N); refined distances are 0.870 (16) and 0.851 (16) Å. Other H atoms were placed in calculated positions, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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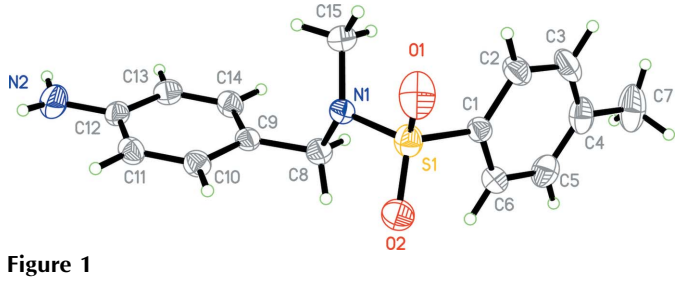

Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

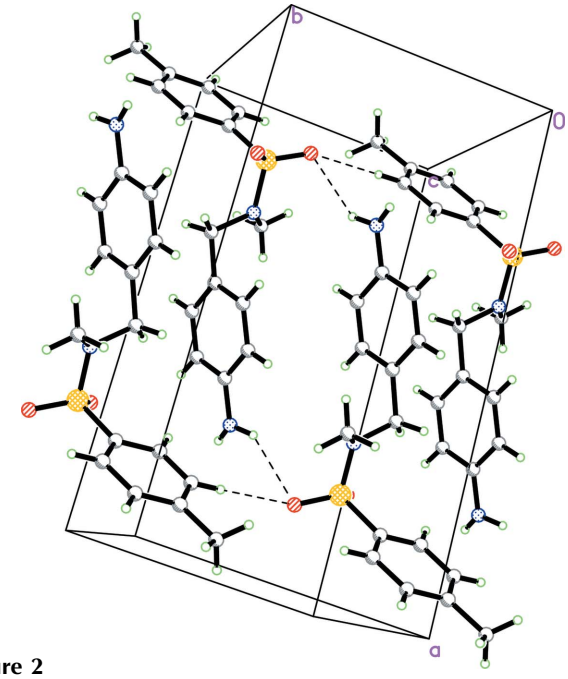

Figure 2
Part of the crystal structure of (I), with hydrogen bonds shown as dashed lines.

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