

4-Methyl-*N*-(4-nitrophenyl)benzenesulfonamide

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In the molecule of the title compound, $C_{13}H_{12}N_2O_4S$, the two benzene ring planes are nearly orthogonal to one another [dihedral angle = $86.1(1)^\circ$]. The C—N—S—C torsion angle in the central part of the molecule is $65.85(13)^\circ$. The molecular packing is stabilized by intermolecular N—H \cdots O interactions.

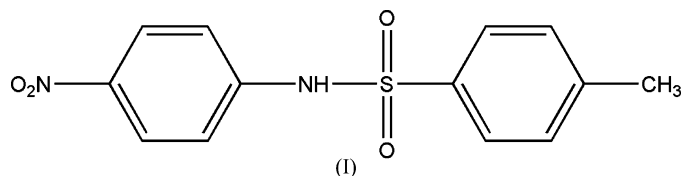
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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(C-C) = 0.002\text{ \AA}$
 R factor = 0.037
 wR factor = 0.120
Data-to-parameter ratio = 16.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Comment

Derivatives of $p-(O_2N)C_6H_4NHSO_2C_6H_4-p-Me$ have been used as starting materials for drugs, such as antagonists of the neurotensin receptors (Labeuw *et al.*, 1996) and microbicide compositions for agriculture and horticultural use (Takanori *et al.*, 2002). In addition, it has also been used to prepare dyes (Bugaut *et al.*, 1981).



The molecular structure of the title compound, (I), is illustrated in Fig. 1 and selected bond distances and angles are given in Table 1. The benzene ring of the nitrophenyl moiety is almost perpendicular to that of the *p*-toluenesulfonamide moiety, making a dihedral angle of $86.1(1)^\circ$. In the crystal structure, the molecules stack along the *b*-axis direction and adjacent molecules are linked *via* N—H \cdots O hydrogen bonds (Table 2 and Fig. 2).

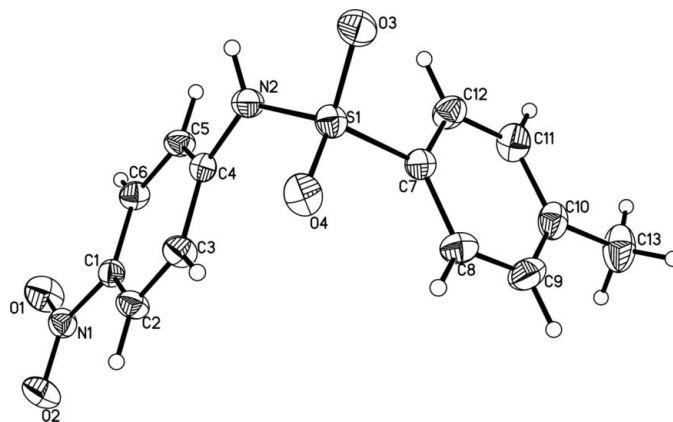


Figure 1

A view of the molecular structure of compound (I), showing the atom-numbering scheme, with displacement ellipsoids drawn at the 30% probability level.

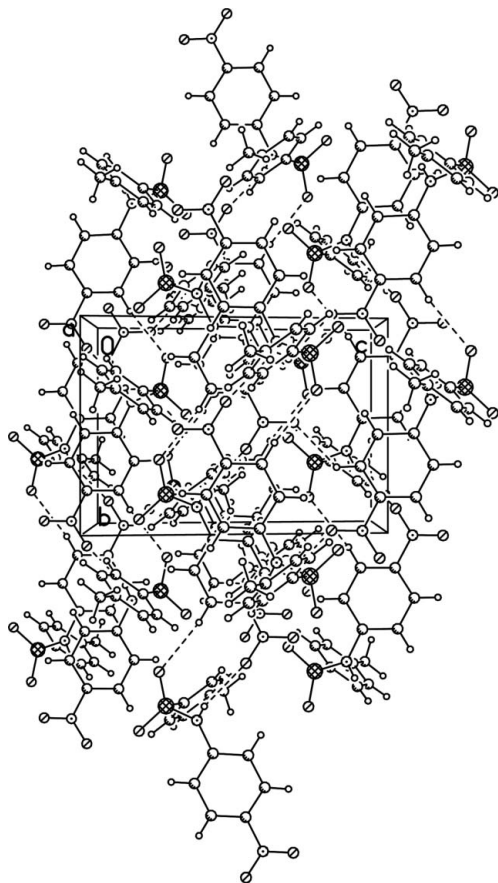


Figure 2

The crystal packing of compound (I), viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

Experimental

The title compound was prepared according to the method described by Bekar *et al.* (1964). To a stirred solution of 13.8 g (0.1 mol) of *p*-nitroaniline in 50 ml of pyridine, 21.0 g (0.11 mol) of *p*-tolylsulfonyl chloride was added. The mixture was heated on a steam-bath for 30 minutes, protected from moisture. Dilution of the hot reaction mixture with 150 ml of 50% ethanol and chilling gave 27.1 g (93%) of compound (I). Recrystallization from ethanol gave light-yellow crystals, m.p. 465–467 K.

Crystal data

$C_{13}H_{12}N_2O_4S$
 $M_r = 292.31$
 Monoclinic, $P2_1/c$
 $a = 13.800$ (3) Å
 $b = 8.2320$ (16) Å
 $c = 11.959$ (2) Å
 $\beta = 103.36$ (3)°
 $V = 1321.8$ (5) Å³
 $Z = 4$

$D_x = 1.469$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 12625 reflections
 $\theta = 3.0$ – 27.5°
 $\mu = 0.26$ mm⁻¹
 $T = 293$ (2) K
 Block, light-yellow
 $0.59 \times 0.45 \times 0.31$ mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
 oscillation scans
 Absorption correction: empirical (using intensity measurements) (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.861$, $T_{\max} = 0.924$
 12625 measured reflections

3031 independent reflections
 2669 reflections with $I > 2I$
 $R_{\text{int}} = 0.031$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -17 \rightarrow 17$
 $k = -10 \rightarrow 10$
 $l = -15 \rightarrow 15$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.120$
 $S = 1.02$
 3031 reflections
 182 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0789P)^2 + 0.2786P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.043$
 $\Delta\rho_{\text{max}} = 0.38$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.055 (4)

Table 1

Selected geometric parameters (Å, °).

S1–O3	1.4298 (12)	N1–O1	1.2141 (18)
S1–N2	1.6360 (13)	N2–C4	1.4118 (17)
S1–C7	1.7597 (15)	C3–C4	1.3938 (19)
O4–S1–O3	120.08 (7)	C4–N2–S1	126.64 (10)
N2–S1–C7	106.06 (7)	C2–C1–N1	119.27 (12)
O1–N1–O2	122.52 (13)	C9–C10–C13	120.99 (18)
O1–N1–C1–C2	176.11 (15)	N2–S1–C7–C8	–122.62 (13)
O1–N1–C1–C6	–1.6 (2)	O3–S1–C7–C12	–52.36 (14)
S1–N2–C4–C3	37.13 (19)	N2–S1–C7–C12	59.12 (13)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2–H2A \cdots O2 ⁱ	0.86	2.30	2.9672 (18)	135

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

All H atoms were positioned geometrically and refined using a riding model, with C–H 0.97 Å, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for Me H atoms].

Data collection: RAPID-AUTO (Rigaku, 2004); cell refinement: RAPID-AUTO; data reduction: RAPID-AUTO; 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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