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N-tert-Butyl-4-toluenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.109
Data-to-parameter ratio = 19.4

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

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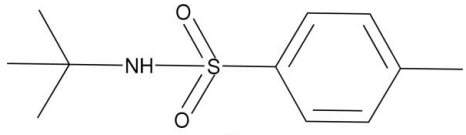
Molecules of the title compound, $C_{11}H_{17}NO_2S$, are linked by paired N—H···O hydrogen bonds into centrosymmetric $R_2^2(8)$ dimers.

Comment

The sulfonamide group is present in many bioactive compounds (Patani & Lavoie, 1996; Thornber, 1979). As the most widely used sulfonamide protecting group is the *tert*-butyl group, *N-tert*-butylarylsulfonamides are usually used as intermediates of sulfonamides (Le Bourdonnec *et al.*, 2000; Murugesan *et al.*, 2003; Graham & Scholz, 1991). We report here the crystal structure of the title compound, (I).



(I)

Bond lengths and angles in (I) are normal. The dihedral angle between the C2–C7 and S1/N1/C11 planes is 80.14 (8)°. The molecules form centrosymmetric dimers *via* N—H···O hydrogen bonds (Table 1 and Fig.2).

Experimental

Aqueous NaOH (7 ml, 10%) was added dropwise to a mixture of 4-toluenesulfonyl chloride (0.58 g) and *tert*-butylamine (1 ml) with constant stirring for 4 h. The solvent was then evaporated in a vacuum. The residue was dissolved in aqueous ethanol and white single crystals of the title compound suitable for X-ray diffraction analysis were obtained by slow evaporation of the solvent.

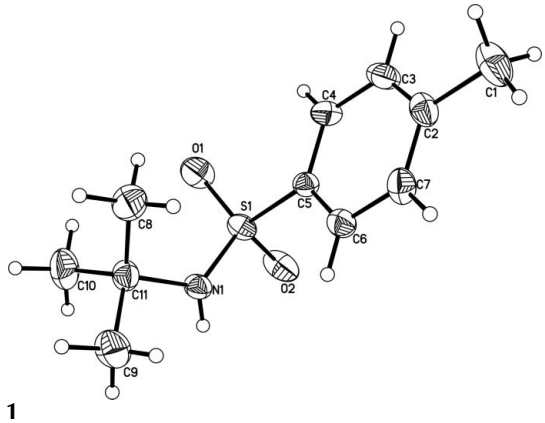


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

Crystal data

$C_{11}H_{17}NO_2S$
M_r = 227.32
Monoclinic, $P2_1/c$
a = 6.1484 (7) Å
b = 24.812 (3) Å
c = 8.1623 (9) Å
β = 97.306 (1)°
V = 1235.1 (2) Å^3
Z = 4
D_x = 1.222 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 291 (2) K
Block, white
0.47 × 0.37 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.895, T_{max} = 0.942
8662 measured reflections
2791 independent reflections
2401 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.109
S = 1.08
2791 reflections
144 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.3046P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.013
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.79 (2)	2.20 (2)	2.982 (2)	170 (2)

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

Atom H1 was located in a difference map and refined isotropically. The remaining H atoms were placed in calculated positions, and refined using a riding model, with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

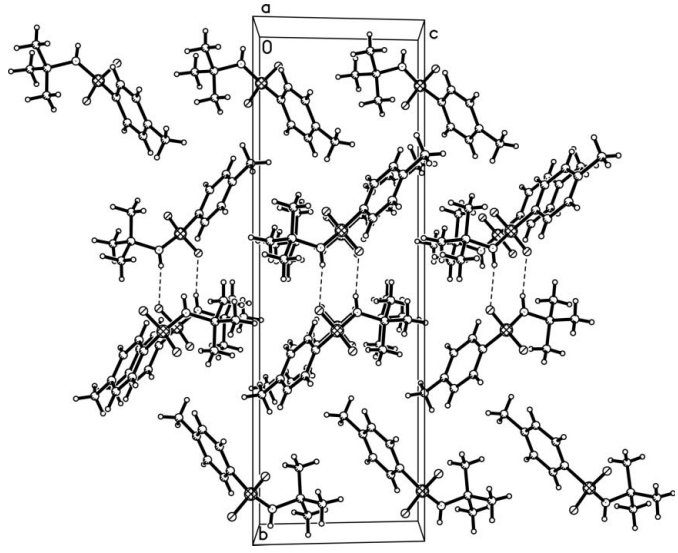


Figure 2
View of the packing along the *a* axis. N—H···O hydrogen bonds are shown as dashed lines.

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