# organic papers

2-(Tosylamino)butan-1-ol

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Key indicators

Single-crystal X-ray study
$T = 293$ K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.116
Data-to-parameter ratio = 19.0

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

In the title compound, $C_{11}H_{17}NO_3S$, the crystal packing is stabilized by O—H···O and N—H···O hydrogen bonds and intermolecular π–π interactions.

Comment

Sulfone, sulfate, thiol, sulfonamide and sulfoxide compounds exhibit insecticidal, antimicrobial and germicidal activitites (Krishnaiah *et al.*, 1995; De Benedetti *et al.*, 1985; Dupont *et al.*, 1978). Sulfur-containing compounds mostly act as simple narcotics (Schultz *et al.*, 2001). The conformation about the S atom determines the pharmacological activity of the compound (McKenna *et al.*, 1989). In view of the importance of this type of compound, we have undertaken the structure determination of the title compound (I), a sulfonamide derivative (Fig. 1 and Table 1).

(I)
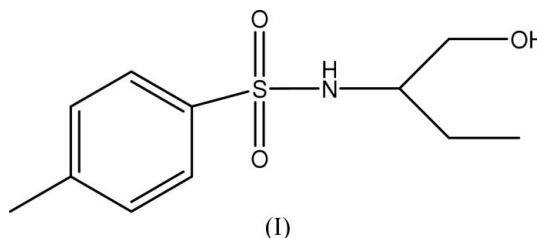
The bond lengths and bond angles are comparable with literature values (Allen *et al.*, 1987). Atom C1 deviates by 0.047 (3) Å from the plane of the benzene ring (C2–C7).

The crystal packing is stabilized by O—H···O and N—H···O hydrogen bonds and intermolecular π–π interactions. Atom O3 acts as a donor to O1, and N1 acts as a donor to O3 (Table 2), generating $R_2^2(14)$ and $R_2^2(10)$ rings, respectively (Bernstein *et al.*, 1995). Atom O3 acts as both a donor and an acceptor, leading to a zigzag chain-like pattern of packing running along the *a* axis. The chains along *a* are further stabilized by π–π interactions, Cg···Cg^i [symmetry code: (i) $1 - x, 1 - y, z$; Cg is the centroid of the C2–C7 ring], with a centroid–centroid separation of 3.885 (1) Å.

Experimental

10% NaOH (5 ml) was added dropwise at 273 K to a solution of 2-aminobutan-1-ol (1 mmol), *p*-toluenesulfonyl chloride (1 mmol) and a catalytic amount of tetrabutylammonium fluoride in benzene (20 ml). The reaction mixture was stirred at room temperature for 10 h, and the organic layer separated, concentrated and column chromatographed to obtain the title compound, which was recrystallized from hexane–ethyl acetate (9:1).
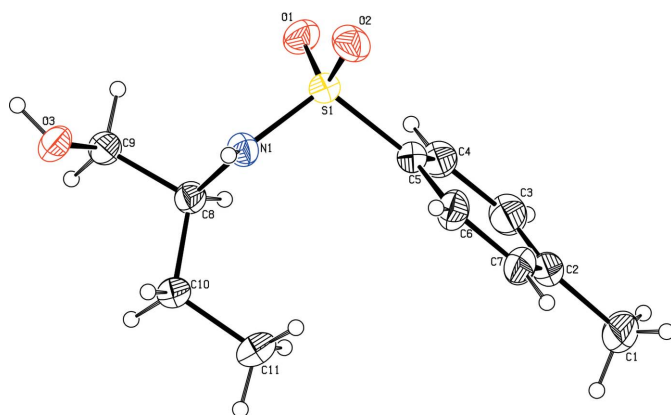
Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

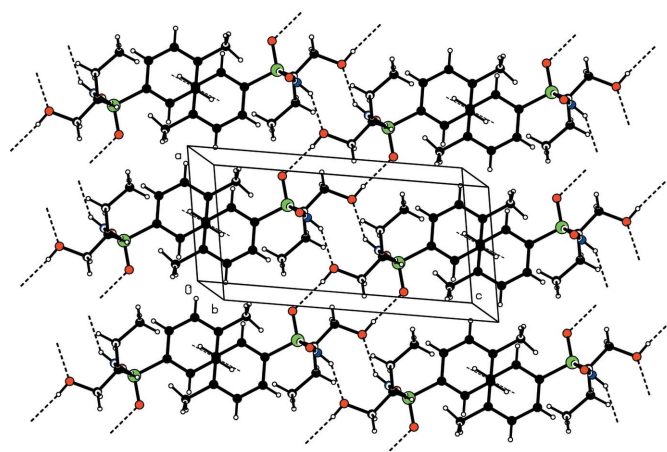**Figure 2**
The molecular packing of (I), viewed approximately along the *b* axis, showing O—H⋯O and N—H⋯O hydrogen bonds, drawn as thick dashed lines, and $\pi-\pi$ interactions, drawn as narrow dashed lines.

Crystal data

$C_{11}H_{17}NO_3S$
$M_r = 243.32$
Triclinic, $P\bar{1}$
$a = 6.4659\ (4)$ Å
$b = 7.0150\ (5)$ Å
$c = 14.2483\ (9)$ Å
$\alpha = 101.720\ (1)°$
$\beta = 97.962\ (1)°$
$\gamma = 99.015\ (1)°$

$V = 615.22\ (7)$ Å^3
$Z = 2$
$D_x = 1.313$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.26$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
$0.26 \times 0.25 \times 0.21$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
7043 measured reflections

2810 independent reflections
2617 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 28.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.116$
$S = 1.04$
2810 reflections
148 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 0.0989P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Table 1
Selected torsion angles (°).

C9—C8—N1—S1	−100.7 (1)	C4—C5—S1—N1	110.5 (1)
C10—C8—N1—S1	135.0 (1)	C6—C5—S1—N1	−69.1 (1)
C8—N1—S1—C5	−72.1 (1)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C4—H4⋯O1	0.93	2.49	2.867 (2)	105
O3—H3A⋯O1^i	0.82	2.02	2.837 (2)	175
N1—H1⋯O3^{ii}	0.86	2.12	2.890 (2)	149

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

All H-atoms were refined using a riding model, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic, C—H = 0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for CH, C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for CH$_2$, C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for CH$_3$, N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(N)$ for NH, and O—H = 0.82 Å and $U_{iso}(H) = 1.5U_{eq}(O)$ for OH.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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* and *PARST* (Nardelli, 1995).

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