Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*S*)-3-Phenyl-2-(tosylamino)propan-1-ol

K. Chinnakali,[a]‡ M. Poornachandran,[b] R. Raghunathan[b] and Hoong-Kun Fun[c]*

[a]Department of Physics, Anna University, Chennai 600 025, India, [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, and [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

‡ Additional correspondence author, email: kali@annauniv.edu

Correspondence e-mail: hkfun@usm.my

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.112
Data-to-parameter ratio = 22.3

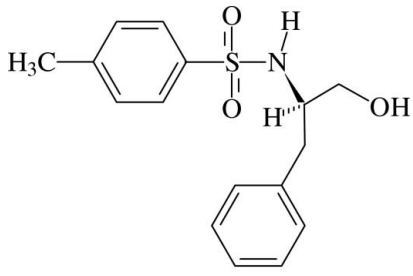
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 28 December 2006
Accepted 23 January 2007

In the title compound, $C_{16}H_{19}NO_3S$, the dihedral angle between the benzene and phenyl rings is 54.17 (6)°. In the crystal structure, the molecules are linked into a two-dimensional network parallel to the (001) plane by N—H···O and O—H···O hydrogen bonds.

Comment

Benzenesulfonamide derivatives have been reported to possess significant biological activities, such as antibacterial (Nieto *et al.*, 2005), anticancer and anti-HIV (Pomarnacka & Kozlarska-Kedra, 2003), antitumor (Yang *et al.*, 2002), and are used as cyclooxygenase-2 (COX-2) inhibitors (Chen *et al.*, 2005). We report here the structure of the title compound, (I), a benzenesulfonamide derivative.



(I)

The geometry of the benzenesulfonamide unit in (I) (Table 1) agrees with that observed in similar structures (Xing *et al.*, 2006; Zareef *et al.*, 2006). The sum of the bond angles around atom N1 (357.8°) indicates sp^2 hybridization. The bond lengths and angles in the aminophenyl-propan-1-ol fragment agree with those reported for (*S*)-*N*-(1-benzyl-2-hydroxy-

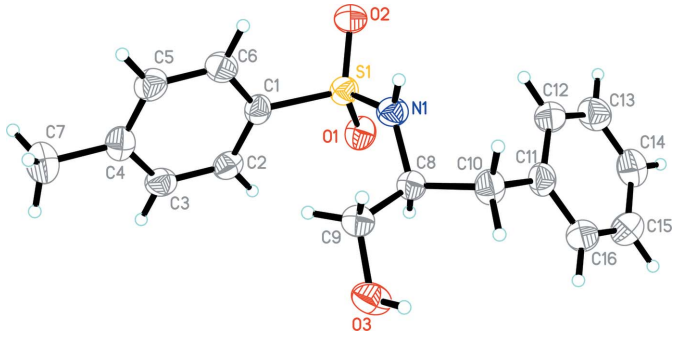


Figure 1
The molecular structure of (I), showing 80% probability displacement ellipsoids and the atomic numbering scheme.

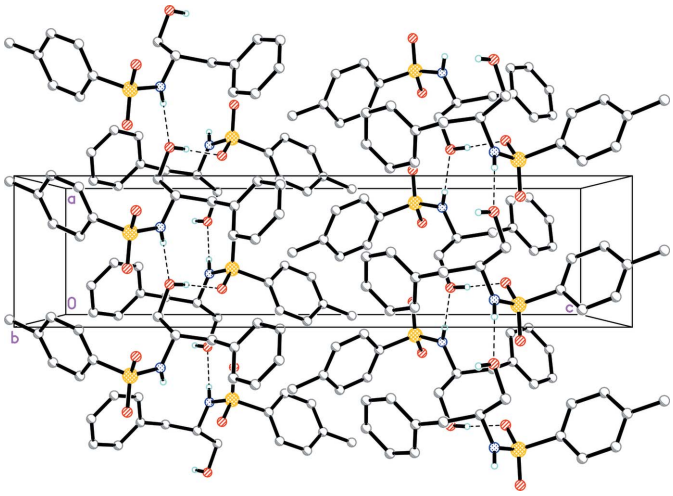


Figure 2
A view of the hydrogen-bonded (dashed lines) network in (I). For clarity, H atoms not involved the network have been omitted.

ethyl)benzamide (Cai *et al.*, 2005). The dihedral angle between the benzene and phenyl rings is 54.17 (6)°.

Molecules translated by one unit along the *a* axis are linked through N1—H1···O3^{i} hydrogen bonds, forming a *C*(6) chain. Screw-related molecules in adjacent chains are cross-linked *via* O3—H3*O*···O1^{ii} hydrogen bonds, forming a two-dimensional network parallel to the (001) plane (Fig. 2). This two-dimensional network is constructed *via* $R_4^4(18)$ motifs. The network structure is further strengthened by weak C—H···O hydrogen bonds, and C—H···π interactions involving the sulfonyl-bound benzene ring; see Table 2 for symmetry codes.

Experimental

NaOH (10%, 5 ml) was added dropwise to a solution of (*S*)-phenylalaninol (1 mmol), *p*-toluenesulfonyl chloride (1 mmol) and a catalytic amount of tetrabutylammonium fluoride in benzene (20 ml) at 273 K. The reaction mixture was stirred at room temprature for 6 h, and the organic layer separated, concentrated and chromatographed to obtain the title compound. Crystals were grown by slow evaporation of a hexane–ethyl acetate (8:2 *v*/*v*) solution.

Crystal data

$C_{16}H_{19}NO_3S$
M_r = 305.38
Orthorhombic, $P2_12_12_1$
a = 5.6735 (1) Å
b = 11.5920 (2) Å
c = 23.2014 (4) Å
V = 1525.89 (5) Å^3
Z = 4
D_x = 1.329 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 100.0 (1) K
Block, colorless
0.25 × 0.16 × 0.10 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.870, T_{max} = 0.979
20899 measured reflections
4447 independent reflections
3743 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 30.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.10
4447 reflections
199 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Absolute structure: Flack (1983), 1840 Friedel pairs
Flack parameter: −0.09 (7)

Table 1
Selected torsion angles (°).

C1—S1—N1—C8	74.69 (18)	C10—C8—C9—O3	−66.8 (2)
N1—S1—C1—C6	71.65 (17)	N1—C8—C10—C11	−77.4 (2)
S1—N1—C8—C10	145.93 (14)	C9—C8—C10—C11	159.27 (18)
S1—N1—C8—C9	−90.75 (19)	C8—C10—C11—C12	71.2 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.84 (3)	2.04 (3)	2.870 (2)	171 (2)
O3—H3*O*···O1^{ii}	0.88 (3)	1.89 (3)	2.770 (2)	175 (3)
C2—H2···O2^{iii}	0.95	2.49	3.152 (2)	126
C10—H10*B*···O1^{ii}	0.99	2.50	3.381 (2)	148
C3—H3···*Cg*1^{iv}	0.95	2.73	3.481 (2)	136

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+1, y, z$; (iv) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$. *Cg*1 is the centroid of the sulfonyl-bound benzene ring.

The imino and hydroxyl H atoms were located in a difference map and refined isotropically. The remaining H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H = 0.95–1.00 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.2U_{eq}(methyl C). A rotating-group model was used for the methyl group.

Data collection and cell refinement: *APEX2* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2005); program(s) used to solve and refine structure: *SHELXTL* (Sheldrick, 1998); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

HKF thanks the Malaysian Government and Universiti Sains Malaysia for Scientific Advancement Grant Allocation (SAGA) grant No. 304/PFIZIK/653003/A118 and USM short-term grant No. 304/PFIZIK/635028.

References

Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12A) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Cai, Y.-M., Fang, H., Jin, Y., Zeng, Q.-L. & Zhao, Y.-F. (2005). *Acta Cryst.* E**61**, o3912–o3913.
Chen, Q. H., Rao, P. N. & Knaus, E. E. (2005). *Bioorg. Med. Chem.* **13**, 2459–2468.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Nieto, M. J., Alovero, F. L., Manzo, R. H. & Mazzieri, M. R. (2005). *Eur. J. Med. Chem.* **40**, 361–369.
Pomarnacka, E. & Kozlarska-Kedra, I. (2003). *Il Farmaco*, **58**, 423–429.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Xing, J.-D., Bai, G.-Y., Zeng, T. & Li, J.-S. (2006). *Acta Cryst.* E**62**, o79–o80.
Yang, L. M., Lin, S. J., Hsu, F. L. & Yang, T. H. (2002). *Bioorg. Med. Chem. Lett.* **12**, 1013–1015.
Zareef, M., Iqbal, R., Zaidi, J. H., Arfan, M. & Parvez, M. (2006). *Acta Cryst.* E**62**, o2481–o2483.