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(1*R*,2*S*)-2-[*N*-Methyl-*N*-(4-toluenesulfonyl)amino]-1-phenylpropan-1-ol

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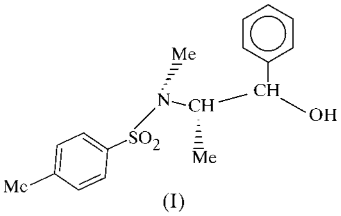
In the title compound, $C_{17}H_{21}NO_3S$, the S atom is in a distorted tetrahedral geometry and the N atom exhibits sp^2 character. The antiperiplanar conformation is observed for the N and hydroxyl-O atoms and the torsion angle around the N—C linkage is −136.3 (2)°. The molecules are linked by O—H···O intermolecular hydrogen bonds to form an infinite one-dimensional chains along the *c* axis.

Comment

The title compound is an *N*-tosyl derivative of (−)-ephedrine. Generally ephedrine and its derivatives are used as sympathomimetic agents for allergic disorders, central nervous system stimulation, prophylaxis and treatment of hypotension and hypersensitive carotid sinus. The structure determination of the title compound, (I), was carried out in order to elucidate the molecular conformation and packing arrangements.



(I)

The S atom is in a distorted tetrahedral geometry with the maximum and minimum bond angles around this atom being 119.8 (1) and 106.4 (1)°, respectively. The sum of the bond angles around the N1 atom [354.6 (2)°] indicates the sp^2 character of this atom; the deviation of N1 from the S1–C8–C9 plane is 0.206 (2) Å. The S—N, S—O and C—S distances agree with those values reported for the toluenesulfonylamino derivatives (Urtiaga *et al.*, 1994; Arriortua *et al.*, 1995).

The N1—C9—C11—O3 torsion angle [164.6 (2)°], characterizes the antiperiplanar conformation for the N1 and O3 atoms. The conformation observed across the S1—N1—C9—C11 linkage is (−)-anticlinal [torsion angle −136.3 (2)°]. The two phenyl ring planes are at a dihedral angle of 59.3 (1)° (see Fig. 1).

In the solid state, the molecules translated in the *c* direction are linked through O3—H3*B*···O2^{i} intermolecular hydrogen bonds (Table 2) to form infinite one-dimensional chains. Along the chain, the phenyl rings are stacked without any π–π interactions.

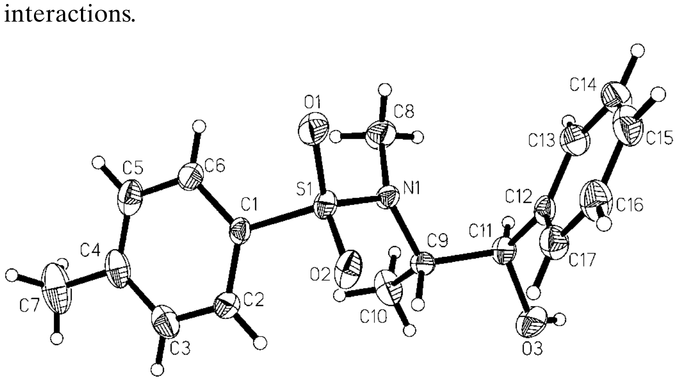


Figure 1
The structure of title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

Ephedrine (1 g, 6.05 mmol), *p*-toluenesulfonyl chloride (1.73 g, 9.07 mmol) and tetra-*n*-butylammonium hydrogen sulfate (0.410 g, 1.21 mmol) in 50 ml of dry benzene were stirred with 10 ml of 50% NaOH at room temperature for 1 h. After completion of the reaction, the organic layer was separated, washed with water and dried over $MgSO_4$. After removal of the solvent, it gave a solid which was recrystallized from methyl alcohol (yield 80%, m.p. 397–399 K).

Crystal data

$C_{17}H_{21}NO_3S$
$M_r = 319.41$
Monoclinic, $P2_1$
$a = 6.0272$ (2) Å
$b = 18.6624$ (8) Å
$c = 7.3642$ (3) Å
$\beta = 98.148$ (1)°
$V = 819.98$ (6) Å^3
$Z = 2$
$D_x = 1.294$ Mg m^{-3}

D_m not measured
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 4453 reflections
$\theta = 2.79$–33.14°
$\mu = 0.209$ mm^{-1}
$T = 293$ (2) K
Parallelepiped, colourless
0.50 × 0.34 × 0.26 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.903$, $T_{max} = 0.948$
5485 measured reflections

3379 independent reflections
3038 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.50°$
$h = -7 \rightarrow 7$
$k = -24 \rightarrow 24$
$l = 0 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.104$
$S = 1.060$
3379 reflections
199 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 0.0071P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter = 0.13 (7)

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Table 1
Selected geometric parameters (Å, °).

S1—O1	1.425 (2)	N1—C9	1.475 (3)
S1—O2	1.434 (2)	O3—C11	1.427 (3)
S1—N1	1.629 (1)	C9—C11	1.540 (3)
S1—C1	1.771 (2)	C11—C12	1.505 (3)
N1—C8	1.461 (3)		
O1—S1—O2	119.9 (1)	N1—S1—C1	108.5 (1)
O1—S1—N1	107.2 (1)	C8—N1—C9	118.4 (2)
O2—S1—N1	107.2 (1)	C8—N1—S1	116.7 (2)
O1—S1—C1	106.4 (1)	C9—N1—S1	119.5 (1)
O2—S1—C1	107.2 (1)		
O1—S1—N1—C9	164.4 (2)	S1—N1—C9—C10	98.6 (2)
C1—S1—N1—C9	−81.0 (2)	S1—N1—C9—C11	−136.3 (2)
O1—S1—C1—C6	20.8 (2)	N1—C9—C11—O3	164.6 (2)
O2—S1—C1—C2	−31.4 (2)		

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 1990).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*B*···O2^{i}	0.82	2.27	3.047 (2)	158

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

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: HA1248). Services for accessing these data are described at the back of the journal.

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