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2-[*N*-(Prop-2-ynyl)-*N*-tosylamino]ethanol

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.001 Å
R factor = 0.036
wR factor = 0.101
Data-to-parameter ratio = 40.0

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

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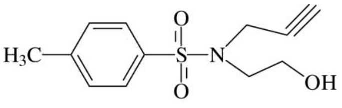
Molecules of the title compound, $C_{12}H_{15}NO_3S$, are linked by a pair of O—H···O hydrogen bonds, forming a centrosymmetric $R_2^2(14)$ dimer. The dimers are cross-linked by a pair of C—H···O hydrogen bonds, forming a ribbon along the *a* axis.

Comment

Benzenesulfonamide derivatives inhibit proliferation of colon adenocarcinoma cells (Kusunoki *et al.*, 2006) and are used as cyclooxygenase-2 (COX-2) inhibitors (Tsai *et al.*, 2006). They also exhibit antibacterial (Nieto *et al.*, 2005), anticancer and anti-HIV (Pomarnacka & Kozlarska-Kedra, 2003) activities. We report here the structure of the title compound, (I).



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles in the benzenesulfonamide unit (Table 1) agree with those reported for similar structures (Xing *et al.*, 2006; Zareef *et al.*, 2006). The sum of the bond angles around atom N1 (349.2°) indicates sp^3 hybridization.

Weak O—H···N and C—H···O interactions are observed in the molecular structure. In the solid state, the molecules are linked by a pair of O3—H3*O*···O1^{i} hydrogen bonds, forming a centrosymmetric $R_2^2(14)$ dimer. The dimers translated by a unit cell along the *a* axis are linked by a pair of C10—H10···O3^{ii} hydrogen bonds, forming a ribbon (Fig. 2); see Table 2 for symmetry codes.

Experimental

Propargyl bromide (1.2 mmol) was added dropwise to a solution of *N*-tosylaminoethanol (1 mmol) and anhydrous potassium carbonate

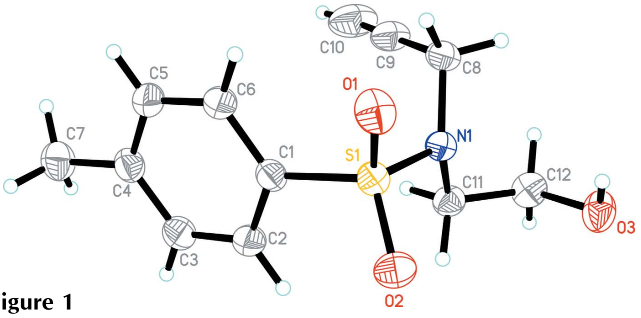


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 80% probability level.

(1.5 mmol) in dry acetone (20 ml). The mixture was stirred until the reaction was complete, as indicated by thin-layer chromatography. The reaction mixture was filtered. The filtrate was evaporated *in vacuo* and column chromatographed with a hexane–ethyl acetate (8:2) mixture to obtain the title compound. Crystals suitable for X-ray analysis were grown by slow evaporation of an ethyl acetate solution.

Crystal data

$C_{12}H_{15}NO_3S$
$M_r = 253.31$
Monoclinic, $P2_1/c$
$a = 8.3174$ (2) Å
$b = 20.3109$ (4) Å
$c = 7.4333$ (1) Å
$\beta = 97.897$ (1)°
$V = 1243.83$ (4) Å^3
$Z = 4$
$D_x = 1.353$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.26$ mm^{-1}
$T = 100.0$ (1) K
Block, colourless
0.51 × 0.44 × 0.42 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.803$, $T_{max} = 0.899$
26785 measured reflections
6524 independent reflections
5480 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 37.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.101$
$S = 1.05$
6524 reflections
163 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 0.279P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.4354 (6)	N1—C11	1.4749 (10)
S1—O1	1.4380 (6)	N1—C8	1.4800 (9)
S1—N1	1.6403 (7)	C8—C9	1.4687 (11)
S1—C1	1.7580 (8)	C9—C10	1.1962 (12)
O3—C12	1.4220 (10)		
O2—S1—O1	119.71 (4)	C11—N1—S1	115.87 (5)
C11—N1—C8	116.06 (6)	C8—N1—S1	117.22 (5)
C1—S1—N1—C11	−67.39 (6)	S1—N1—C11—C12	−153.11 (5)
C1—S1—N1—C8	75.60 (6)	N1—C11—C12—O3	61.93 (8)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*O*···N1	0.85 (1)	2.62 (1)	2.9363 (9)	103 (1)
O3—H3*O*···O1^{i}	0.85 (1)	1.99 (1)	2.8227 (9)	166 (1)
C6—H6···O1	0.95	2.56	2.9258 (11)	103
C8—H8*A*···O1	0.99	2.36	2.8732 (10)	111
C10—H10···O3^{ii}	0.96 (2)	2.38 (2)	3.2457 (12)	150 (1)
C11—H11*B*···O2	0.99	2.44	2.9151 (10)	109

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

The propyne and hydroxyl H atoms were located in a difference map and refined isotropically. The C-bound H atoms were positioned geometrically and treated as riding on their parent C atoms, with C—H = 0.95–0.99 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.

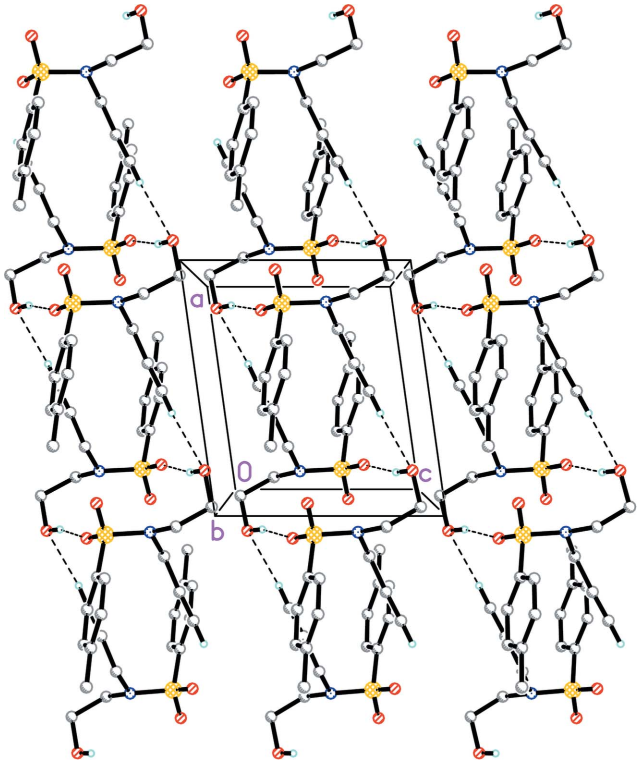


Figure 2
A view of the hydrogen-bonded (dashed lines) ribbon in (I). For the sake of clarity, H atoms not involved in the motif have been omitted.

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

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