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Propane-1,3-diyl bis(*p*-toluenesulfonate)

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In the title compound, $C_{17}H_{20}O_6S_2$, the molecule lies on a twofold rotation axis.

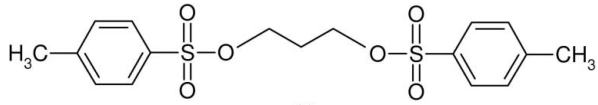
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.056
wR factor = 0.123
Data-to-parameter ratio = 17.6

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

Comment

The title compound, (I), has been reported as an intermediate in the synthesis of cyclic amines (Smith *et al.*, 1978) and as a bridge reagent linking two cyclic amine rings (Wieghardt *et al.*, 1985). In the crystal structure, the molecule adopts a W conformation, with atom C9 lying on a crystallographic twofold rotation axis (Fig. 1). The dihedral angle between the two benzene rings is 83.0 (1)°.



(I)

Experimental

Toluene-4-sulfonyl chloride (30 mg) and 1,3-propanedial (6 g) were dissolved in toluene (180 ml). Triethylamine (19 g) were then added in small amounts with stirring at 263 K. This solution was stirred mechanically at 268 K for 5 h, after which time the resulting white precipitate was filtered off, washed with water and recrystallized from ethanol. Crystals suitable for X-ray analysis were obtained by diffusion of diethyl ether into an ethanol solution over two weeks.

Crystal data

$C_{17}H_{20}O_6S_2$
M_r = 384.45
Monoclinic, $C2/c$
a = 14.8505 (19) Å
b = 5.4005 (7) Å
c = 23.582 (3) Å
β = 100.824 (2)°
V = 1857.6 (4) Å^3
Z = 4
D_x = 1.375 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 292 (2) K
Prism, colourless
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.940, T_{max} = 0.963
5488 measured reflections
2020 independent reflections
1152 reflections with $I > 2\sigma(I)$
R_{int} = 0.085
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.123
S = 0.90
2020 reflections
115 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.028
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

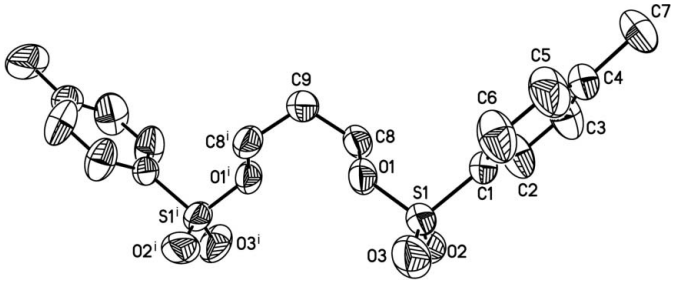


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted. [Symmetry code: (i) $1-x, y, \frac{1}{2}-z$.]

H atoms were positioned geometrically and allowed to ride, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for Csp^2, with C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for the methylene groups, and with C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for the methyl group.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Bruker (2000). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2002). *SADABS*. Version 2.03. University of Göttingen, Germany.
Smith, W. L., Ekstrand, J. D. & Raymond, K. N. (1978). *J. Am. Chem. Soc.* **100**, 3539–3544.
Wieghardt, K., Tolksdorf, I. & Herrmann, W. (1985). *Inorg. Chim.* **24**, 1230–1235.