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N,N'-{[Ethane-1,2-diylbis(oxy)]bis-(ethane-2,1-diyl)}bis(4-methylbenzene-sulfonamide)

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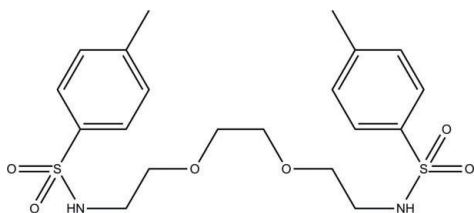
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.053; wR factor = 0.150; data-to-parameter ratio = 14.2.

The asymmetric unit of the title compound, $\text{C}_{20}\text{H}_{28}\text{N}_2\text{O}_6\text{S}_2$, contains one half-molecule, related to the other half by a twofold rotation axis. The two aromatic rings of the molecule make a dihedral angle of $50.91(7)^\circ$. The $\text{O}-\text{CH}_2-\text{CH}_2-\text{O}$ and $\text{N}-\text{CH}_2-\text{CH}_2-\text{O}$ fragments both adopt *gauche* conformations, with torsion angles of $76.0(4)$ and $70.4(3)^\circ$, respectively. In the crystal, adjacent molecules are linked through $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into chains along the *a*-axis direction. The chains are further connected *via* $\text{C}-\text{H}\cdots\text{O}$ interactions into a two-dimensional supramolecular network in the *ac* plane.

Related literature

 For similar structures, see: Polyakova *et al.* (1990); Ding *et al.* (2003).


Experimental

Crystal data

 $\text{C}_{20}\text{H}_{28}\text{N}_2\text{O}_6\text{S}_2$
 $M_r = 456.56$

 Monoclinic, $C2/c$
 $a = 11.135(7)$ Å
 $b = 9.220(6)$ Å
 $c = 21.452(15)$ Å
 $\beta = 93.680(12)^\circ$
 $V = 2198(3)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.28$ mm⁻¹
 $T = 296$ K
 $0.23 \times 0.14 \times 0.04$ mm

Data collection

 Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.938$, $T_{\max} = 0.989$

 5135 measured reflections
 1983 independent reflections
 1558 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.055$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.150$
 $S = 1.03$
 1983 reflections
 140 parameters
 1 restraint

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.32$ e Å⁻³
 $\Delta\rho_{\min} = -0.36$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1 \cdots O2 ⁱ	0.82 (2)	2.14 (2)	2.944 (3)	171 (3)
C6—H6 \cdots O1 ⁱⁱ	0.93	2.56	3.311 (4)	138

 Symmetry codes: (i) $-x + 1, y, -z + \frac{3}{2}$; (ii) $-x + 1, -y, -z + 1$.

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: SHELXL97 and publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2551).

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