

(E)-N'-(9-Anthrylmethylidene)-p-toluene-sulfonohydrazide

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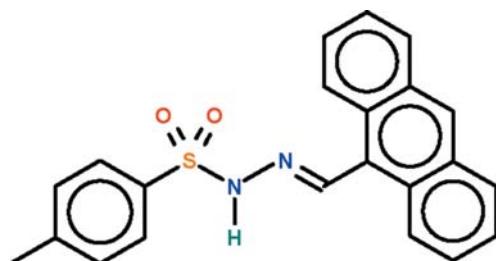
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Key indicators: single-crystal X-ray study; $T = 100\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$; R factor = 0.040; wR factor = 0.104; data-to-parameter ratio = 16.9.

The S—N(H)—N=C linkage in the title molecule, $\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_2\text{S}$, is non-planar [torsion angle = $30.6(1)^\circ$] as the amino N atom is pyramidal coordinated. In the crystal, the amino group acts as a hydrogen-bond donor to an O atom of an adjacent molecule, generating chains running parallel to the b axis.

Related literature

For the structure of the (E)-N'-benzylidene-p-toluenesulfonohydrazide analog, see: Mehrabi *et al.* (2008).

**Experimental***Crystal data*

$\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_2\text{S}$

$M_r = 374.44$

Orthorhombic, $Pbca$
 $a = 17.3634(15)\text{ \AA}$
 $b = 9.2438(8)\text{ \AA}$
 $c = 22.882(2)\text{ \AA}$
 $V = 3672.6(6)\text{ \AA}^3$

$Z = 8$
Mo $K\alpha$ radiation
 $\mu = 0.20\text{ mm}^{-1}$
 $T = 100\text{ K}$
 $0.40 \times 0.20 \times 0.05\text{ mm}$

Data collection

Bruker SMART APEX
diffractometer
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
 $T_{\min} = 0.926$, $T_{\max} = 0.990$

22220 measured reflections
4209 independent reflections
3158 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.055$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.104$
 $S = 1.02$
4209 reflections
249 parameters
1 restraint

H atoms treated by a mixture of
independent and constrained
refinement
 $\Delta\rho_{\max} = 0.34\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.46\text{ e \AA}^{-3}$

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N1—H1 \cdots O1 ⁱ	0.86 (1)	2.07 (1)	2.911 (2)	169 (2)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2262).

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