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(*E*)-*N*′-(2-Thienylmethylidene)-*p*-toluenesulfonohydrazide

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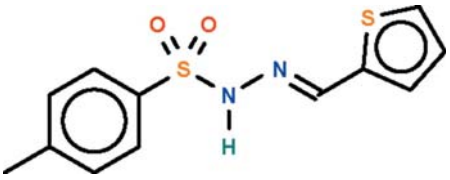
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.085; data-to-parameter ratio = 18.0.

The S—N(H)—N=C linkage in the title molecule, $C_{12}H_{12}N_2O_2S_2$, is non-planar [torsion angle = 15.5 (1)°] as the amino N atom is pyramidally coordinated. The amino group acts as a hydrogen-bond donor to an O atom of an adjacent molecule, generating chains running parallel to the *c* axis.

Related literature

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



Experimental

Crystal data

$C_{12}H_{12}N_2O_2S_2$
M_r = 280.36
Monoclinic, $P2_1/c$
a = 14.3758 (10) Å
b = 9.8613 (7) Å
c = 9.6172 (7) Å
β = 104.981 (1)°
V = 1317.03 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 100 K
0.40 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.857, T_{max} = 0.925
8238 measured reflections
3022 independent reflections
2728 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.085
S = 1.04
3022 reflections
168 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86 (1)	2.06 (1)	2.874 (2)	159 (2)

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

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: PK2261).

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