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2-[(1,3-Benzodioxol-5-ylmethylidene)-amino]-4,5,6,7-tetrahydro-1-benzothiophene-3-carbonitrile

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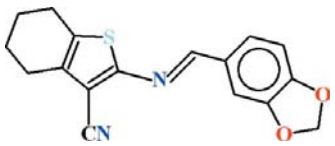
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.119; data-to-parameter ratio = 13.4.

The title compound, $C_{17}H_{14}N_2O_2S$, crystallizes with two roughly planar molecules in the asymmetric unit, in which the dihedral angles between the 1,3-benzodioxole-5-carbaldehyde moiety and the heterocyclic five-membered ring are 3.76 (5) and 5.33 (12)°. In each molecule, a short C—H···S contact generates an S(5) ring. In the crystal, pairs of molecules are linked by a weak C—H···N interaction, forming dimers.

Related literature

For a related structure, see: Elerman & Elmali, (1998). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{17}H_{14}N_2O_2S$
M_r = 310.36
Triclinic, $P\overline{1}$
a = 10.9450 (3) Å
b = 10.9895 (3) Å
c = 13.5749 (3) Å
α = 99.409 (1)°
β = 109.707 (1)°
γ = 92.854 (1)°
V = 1506.77 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 296 K
0.32 × 0.23 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.947, T_{max} = 0.962
21604 measured reflections
5331 independent reflections
3812 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.119
S = 1.01
5331 reflections
397 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···S1	0.93	2.65	3.081 (2)	109
C25—H25···S2	0.93	2.61	3.060 (2)	110
C7—H7A···N4^{i}	0.97	2.62	3.190 (3)	118

Symmetry code: (i) $x, y-1, z$.

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: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6325).

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