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

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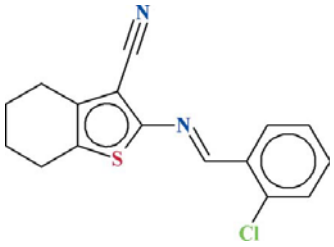
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.105; data-to-parameter ratio = 14.4.

In the title compound, $C_{16}H_{13}ClN_2S$, the mean planes fitted through all non-H atoms of the heterocyclic five-membered and the benzene rings are oriented at a dihedral angle of 5.19 (7)°. In the crystal, a weak C—H$\cdots\pi$ interaction occurs, along with weak π–π interactions [cenroid–centroid distance = 3.7698 (11) Å].

Related literature

For information on the use of Schiff bases in pharmaceutical chemistry, see: Lewinski *et al.* (2005). For related structures, see: Asiri *et al.* (2011*a*,*b*).



Experimental

Crystal data

$C_{16}H_{13}ClN_2S$
M_r = 300.79
Triclinic, $P\overline{1}$
a = 8.3383 (4) Å
b = 8.6885 (4) Å
c = 10.5746 (5) Å
α = 85.975 (2)°
β = 80.806 (2)°
γ = 73.003 (2)°
V = 723.00 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 296 K
0.40 × 0.25 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.931, T_{max} = 0.951
10003 measured reflections
2600 independent reflections
2308 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.105
S = 1.03
2600 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

Cg is the centroid of the C11–C16 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$A\cdots Cg^{i}$	0.97	2.87	3.744 (3)	151

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: NK2106).

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