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

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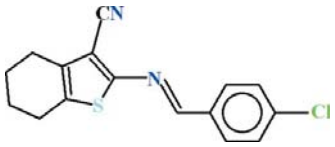
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.099; data-to-parameter ratio = 14.4.

In the title compound, $C_{16}H_{13}ClN_2S$, the dihedral angle between the 4-chlorobenzaldehyde moiety and the heterocyclic five-membered ring is 7.21 (17)°. In the crystal, molecules are linked by weak C—H···π interactions, generating [100] chains.

Related literature

For a related structure, see: Asiri *et al.* (2011).



Experimental

Crystal data

$C_{16}H_{13}ClN_2S$
M_r = 300.79
Orthorhombic, $P2_12_12_1$
a = 4.7815 (3) Å
b = 16.5670 (13) Å
c = 18.1658 (14) Å
V = 1439.01 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 296 K
0.35 × 0.15 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.931, T_{max} = 0.951
11075 measured reflections
2607 independent reflections
1821 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.099
S = 1.02
2607 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 1053 Friedel pairs
Flack parameter: 0.03 (10)

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

Cg is the centroid of the C8–C11/S1 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13A···Cg^i	0.97	2.99	3.841 (6)	147

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

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: HB6331).

References

Asiri, A. M., Khan, S. A. & Tahir, M. N. (2011). *Acta Cryst.* E**67**, o2162.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.