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 <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_{2}S, 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_{2}S
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 Kα 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
R_{int} = 0.055

11075 measured reflections
2607 independent reflections
1821 reflections with I > 2σ(I)

Refinement

R[F^2 > 2σ(F^2)] = 0.044
wR(F^2) = 0.099
S = 1.02
2607 reflections
181 parameters
H-atom parameters constrained
Δρ_{max} = 0.26 e Å^{-3}
Δρ_{min} = −0.19 e Å^{-3}

Absolute structure: Flack (1983), 1053 Friedel pairs
Flack parameter: 0.03 (10)

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

<table>
<thead>
<tr>
<th>D—H···A</th>
<th>D—H</th>
<th>H···A</th>
<th>D···A</th>
<th>D—H···A</th>
</tr>
</thead>
<tbody>
<tr>
<td>C13—H13A···Cg</td>
<td>0.97</td>
<td>2.99</td>
<td>3.841 (6)</td>
<td>147</td>
</tr>
</tbody>
</table>

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: SHELX97 (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


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