Ethyl 3-ethoxycarbonylmethyl-7-methyl-5-phenyl-5H-thiazolo[3,2-a]pyrimidine-6-carboxylate

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Ethyl 3-ethoxycarbonylmethyl-7-methyl-5-phenyl-5H-thiazolo[3,2-a]pyrimidine-6-carboxylate

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Key indicators: single-crystal X-ray study; T = 296 K; mean ϕ(C–C) = 0.002 Å;
R factor = 0.043; wR factor = 0.118; data-to-parameter ratio = 16.1.

In the title compound, C20H22N2O3S, the central pyrimidine ring incorporating a chiral C atom is significantly puckered and adopts a slight boat conformation with C atom bearing the phenyl ring and the N atom opposite displaced by 0.367 (2) and 0.107 (2) Å, respectively, from the plane formed by the remaining ring atoms. The benzene ring is positioned axially to the pyrimidine ring, making a dihedral angle of 88.99 (5)°. The thiazole ring is essentially planar (r.m.s. deviation 0.0033 Å). In the crystal, pairs of C–H···O interactions result in centrosymmetric dimers with graph-set motifs R21(7) and R2(8). A weak C–H···π contact is also observed.

Related literature


Experimental

Crystal data

C20H22N2O3S | a = 10.0861 (4) Å
M = 386.46 | b = 7.7954 (3) Å
Monoclinic, P21/c | c = 23.4088 (10) Å

β = 95.000 (3)°  | μ = 0.21 mm−1
V = 1833.52 (13) Å3  | T = 296 K
Z = 4  | 0.18 × 0.16 × 0.16 mm
Mo Kα radiation

Data collection

Bruker SMART APEX CCD
detector diffractometer
Absorption correction: multi-scan
(SADABS, Bruker, 1998)
Tmin = 0.964, Tmax = 0.968

Refinement

R[F2 > 2σ(F2)] = 0.043
wR(F2) = 0.118
S = 1.00
3982 reflections
247 parameters
H-atom parameters constrained
Δρmax = 0.50 e Å−3
Δρmin = −0.29 e Å−3

Table 1

Hydrogen-bond geometry (Å, °).

Cg is the centroid of the thiazolopyrimidine ring.

<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>C17—H17A···O21</td>
<td>0.97</td>
<td>2.47</td>
<td>3.415 (3)</td>
<td>164</td>
</tr>
<tr>
<td>C5—H5···O21</td>
<td>0.98</td>
<td>2.59</td>
<td>3.429 (2)</td>
<td>144</td>
</tr>
<tr>
<td>C4—H4C···Cg1i</td>
<td>0.96</td>
<td>3.03</td>
<td>3.897 (4)</td>
<td>151</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) −x + 1, −y, −z + 1; (ii) x, −y, −z + 2.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT-Plus (Bruker, 1998); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and CAMERON (Watkin et al., 1996); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2884).

References


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