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2-Cyclohexylamino-5,6-dimethyl-3-phenyl-3*H*-thieno[2,3-*d*]pyrimidin-4(3*H*)-one

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Key indicators

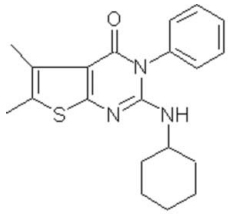
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.138
Data-to-parameter ratio = 16.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

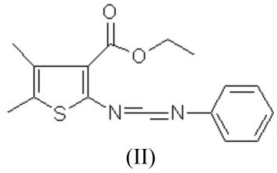
Molecules of the title compound, $C_{20}H_{23}N_3OS$, form a supramolecular structure *via* intermolecular C—H···π interactions.

Comment

Derivatives of thienopyrimidine are of great importance because of their biological properties (Ding et al., 2004). We have recently focused our attention on the synthesis of heterocyclic systems containing a fused pyrimidinone ring using the aza-Wittig reaction (Hu *et al.*, 2005). The title compound, (I), may be used as a new precursor to obtain bioactive molecules. Its structure is reported here (Fig. 1).



(I)



(II)

The bond lengths and angles are unexceptional. The two fused rings are essentially coplanar (Table 1), with maximum deviations of 0.056 (2) and −0.042 (2) Å for C7 and S1, respectively. The dihedral angle between the C15–C20 phenyl ring and the thienopyrimidinone system is 89.00 (1)°. The cyclohexyl ring adopts a distorted chair conformation [φ = 356.64 (2)° and θ = 2.53 (2)°, and puckering amplitude = 0.575 (2) Å; Cremer & Pople, 1975].

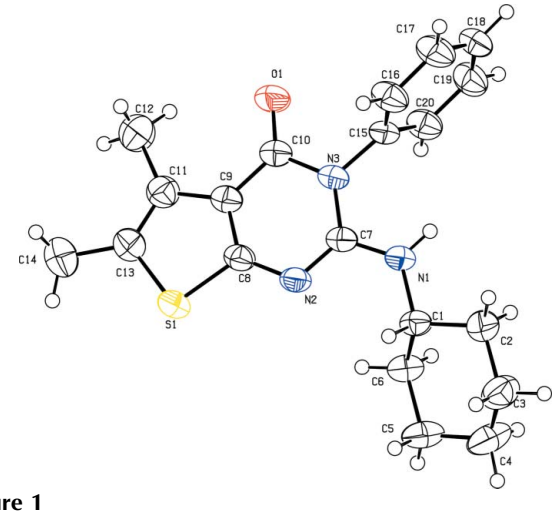


Figure 1
View of the molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

The crystal structure is stabilized by intermolecular C—H···π interactions (Fig. 2 and Table 2)

Experimental

To a solution of (II) (3 mmol) in dichloromethane (15 ml) was added cyclohexylamine (3 mmol). The reaction mixture was allowed to stand for 2 h; the solvent was then removed and anhydrous ethanol (10 ml) with several drops of EtONa in EtOH was added. The mixture was stirred for 5 h at room temperature. The solution was concentrated under reduced pressure and the residue was recrystallized from ethanol to give the title compound. (I) was recrystallized from ethanol–dichloromethane (1:2 *v*/*v*) at room temperature, yielding crystals suitable for single-crystal X-ray diffraction.

Crystal data

$C_{20}H_{23}N_3OS$
M_r = 353.47
Triclinic, $P\overline{1}$
a = 8.813 (3) Å
b = 10.064 (3) Å
c = 11.526 (3) Å
α = 100.522 (5)°
β = 99.819 (5)°
γ = 107.060 (5)°
V = 933.1 (5) Å^3
Z = 2
D_x = 1.258 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 292 (2) K
Block, colorless
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.964, T_{max} = 0.982
5533 measured reflections
3794 independent reflections
3111 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.138
S = 1.04
3794 reflections
228 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0835P)^2 + 0.0173P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected torsion angles (°).

S1—C8—N2—C7	179.00 (11)	N2—C8—S1—C13	−177.06 (14)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the ring S1,C8,C19,C11,C13; *Cg*2 is the centroid of the ring N2,N3,C7–C10.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···*Cg*2^{i}	0.98	2.88	3.62 (2)	133
C2—H2*A*···*Cg*1^{i}	0.97	2.68	3.56 (2)	151
C20—H20···*Cg*2^{ii}	0.93	2.77	3.58 (2)	147

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

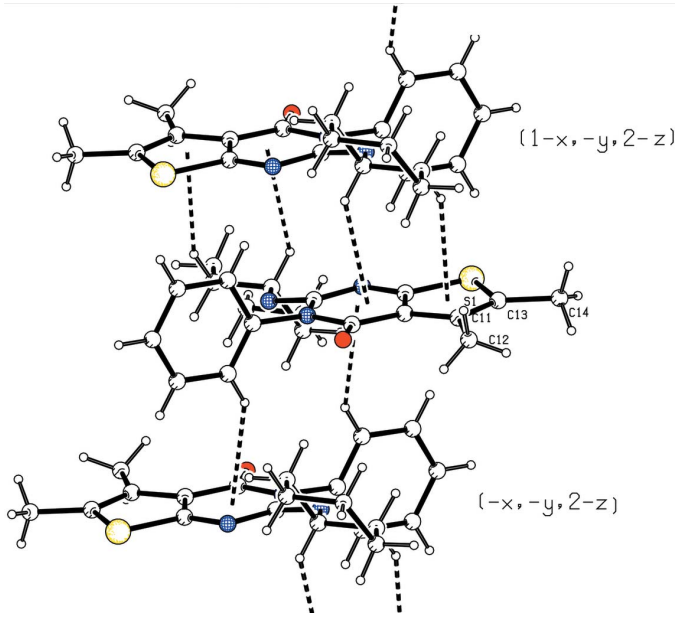


Figure 2
A view of the C—H···π hydrogen-bond stacking interactions (dashed lines).

All H atoms were located in difference maps and treated as riding atoms, with C—H = 0.93 (aromatic), 0.96 (CH_3), 0.97 (CH_2) and 0.98 Å (CH), and N—H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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