Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Ethylamino-3-phenyl-2-benzothieno[3,2-*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
Disorder in main residue
R factor = 0.060
wR factor = 0.162
Data-to-parameter ratio = 15.7

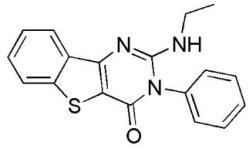
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 24 November 2006
Accepted 28 November 2006

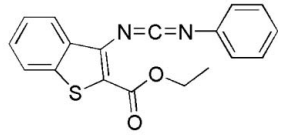
In the title compound, $C_{18}H_{15}N_3OS$, the three fused rings of the benzothienopyrimidinone are essentially coplanar. The crystal structure is stabilized by C—H···O and C—H···S hydrogen bonds.

Comment

Thienopyrimidine derivatives are of interest as possible antiviral agents, and because of their other biological properties, including antibacterial, antifungal, anti-allergic and anti-inflammatory activities (Chambhare *et al.*, 2003). We have recently focused on the synthesis of fused heterocyclic systems containing thienopyrimidine *via* aza-Wittig reactions at room temperature (Ding *et al.*, 2004). We present here the structure of one such thienopyrimidine derivative, the title compound, (I) (Fig. 1).



(I)



(II)

The three fused rings of (I) are essentially coplanar, the maximum deviation from the 2-benzothieno[3,2-*e*]pyrimidi-]pyrimidinone mean plane being 0.033 (3) Å for atom N2. The substituent phenyl ring (C11–C16) is twisted with respect to the ring system, making a dihedral angle of 86.2 (1)°.

In the crystal structure, C—H···O hydrogen bonds link the molecules into rows along the *a* axis. Additional C—H···S

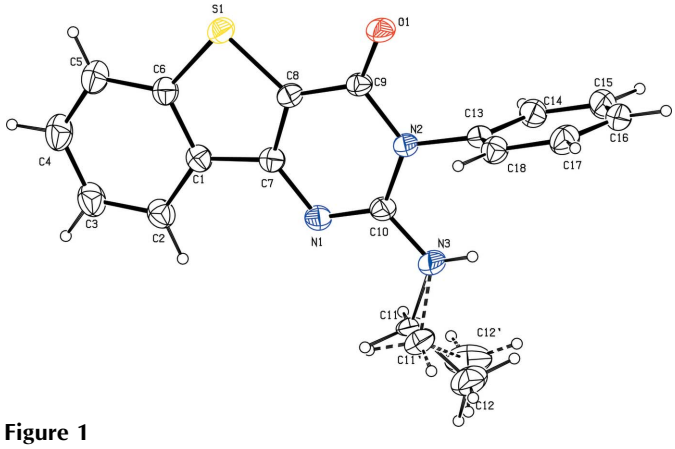


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. Bonds to atoms of the minor disorder component are drawn with dashed lines.

interactions link adjacent rows, giving a network structure (Fig. 2 and Table 1).

Experimental

Ethylamine (3 mmol) was added to a solution of ethyl 3-(phenyliminomethyleneamino)-2-benzothiophene-2-carboxylate, (II) (3 mmol), in dichloromethane (15 ml). After being allowed to stand for 30 min, the solvent was removed and anhydrous ethanol (10 ml) with several drops of EtONa in EtOH was added. The mixture was stirred for 2 h at room temperature, concentrated under reduced pressure and the residue recrystallized from ethanol to give (I). The product was recrystallized from ethanol/dichloromethane (1:2 *v*/*v*) at room temperature to give crystals suitable for single-crystal X-ray diffraction.

Crystal data

$C_{18}H_{15}N_3OS$
M_r = 321.39
Monoclinic, $P2_1/n$
a = 10.2947 (11) Å
b = 12.0592 (13) Å
c = 13.4330 (14) Å
β = 106.599 (2)°
V = 1598.2 (3) Å^3
Z = 4
D_x = 1.336 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 292 (2) K
Block, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
13934 measured reflections
3667 independent reflections
2592 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.162
S = 1.05
3667 reflections
233 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0869P)^2 + 0.0213P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12B···O1^{i}	0.96	2.51	3.322 (6)	142
C15—H15···S1^{ii}	0.93	2.93	3.828 (3)	163

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

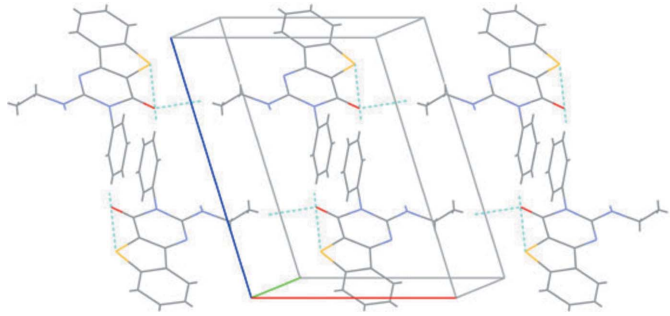


Figure 2
The packing of (I) with hydrogen bonds shown as dashed lines. For clarity, atoms of the minor disorder component of the ethyl group have been omitted.

The ethyl group is disordered over two positions and the final occupancies for the major and minor disorder components refined to 0.512 (14) and 0.488 (14), respectively. Atom H3*A* on N3 was located in a difference Fourier map and refined freely with an isotropic displacement parameter. All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

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* (Bruker, 2001) and *Mercury* (Macrae *et al.*, 2006).

The author acknowledges the National Basic Research Program of China (No. 2004CCA00100) and the National Natural Science Foundation of China (project No. 20102001).

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