organic papers

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.123
Data-to-parameter ratio = 15.6

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

5-Benzyl-6-methyl-2-thioxo-2,3-dihydro-pyrimidin-4(1H)-one

In the title compound, $C_{12}H_{12}N_2OS$, the dihedral angle between the benzene and pyrimidine rings is 84.1 (1)°. The molecules are linked by centrosymmetric pairs of N—H···O [N···O = 2.817 (2) Å] and N—H···S [N···S = 3.357 (2) Å] hydrogen bonds to form chains.

Comment

Pyrimidine derivatives have received much attention due to their versatile uses. They have been widely used as tools to study biochemical systems and as chemotherapeutic agents (Koppel *et al.*, 1961; Furberg & Petersen, 1972). As part of a general programme towards the synthesis of powerful chemotherapeutic agents, the title compound, (I), a new pyrimidine derivative, was synthesized. We report here the crystal structure of (I) (Fig. 1).

(I)
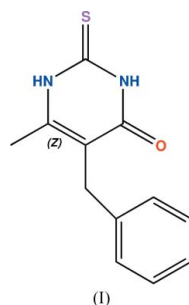
In compound (I), the benzene ring forms a dihedral angle of 84.1 (1)° with the pyrimidine ring. The torsion angles C5—C6—C7—C8 and C6—C7—O8—C9 are 160.0 (2) and 96.4 (3)°, respectively. The C=O and C=S bond lengths are 1.234 (3) and 1.668 (2) Å, respectively. Selected bond lengths and angles are listed in Table 1. The molecules are linked by N—H···O and N—H···S hydrogen bonds (Table 2) to form chains (Fig. 2).

Experimental

The title compound was prepared according to the method described by Craig *et al.* (2000). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution at 283 K

Crystal data

$C_{12}H_{12}N_2OS$	D_x = 1.332 Mg m^{-3}
M_r = 232.30	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 1539
a = 5.8779 (9) Å	reflections
b = 29.800 (4) Å	θ = 2.7–23.4°
c = 7.2160 (11) Å	μ = 0.26 mm^{-1}
β = 113.622 (2)°	T = 292 (2) K
V = 1158.1 (3) Å^3	Block, colourless
Z = 4	0.20 × 0.08 × 0.06 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2274 independent reflections
	1753 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.026$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)	$\theta_{max} = 26.1°$
	$h = -7 \rightarrow 4$
$T_{min} = 0.950$, $T_{max} = 0.985$	$k = -32 \rightarrow 36$
5152 measured reflections	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 0.2016P]$
$R[F^2 > 2\sigma(F^2)] = 0.048$	
$wR(F^2) = 0.123$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
2274 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
146 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C2—N1	1.346 (3)	C5—C8	1.497 (3)
C2—S1	1.668 (2)	C6—C7	1.496 (3)
C4—O1	1.234 (3)	C8—C9	1.508 (3)
C5—C6	1.350 (3)		
N1—C2—N3	114.66 (19)	C5—C6—N1	120.04 (19)
N1—C2—S1	123.03 (16)	C5—C8—C9	116.11 (19)
O1—C4—N3	119.7 (2)	C14—C9—C10	118.2 (2)
O1—C4—C5—C8	−0.2 (3)	C5—C8—C9—C10	160.0 (2)
C6—C5—C8—C9	96.4 (3)	S1—C2—N1—C6	178.81 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1^i	0.86	1.96	2.817 (2)	176
N1—H1···S1^{ii}	0.86	2.51	3.3574 (19)	171

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

The H atoms were placed in idealized positions and constrained to ride on their parent atoms, with N—H distances of 0.86 Å and C—H distances in the range 0.93–0.97 Å [C—H = 0.93 Å for phenyl, C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl, and $U_{iso}(H) = 1.2U_{eq}(C)$ for other H atoms]. The methyl groups were allowed to rotate freely about the C—C bond.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.
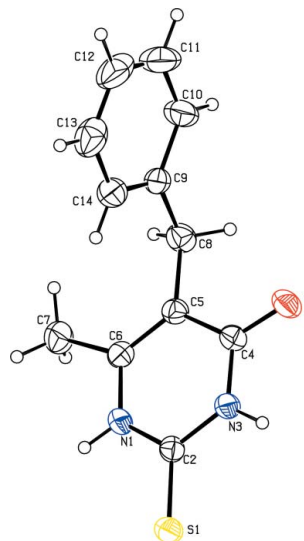
Figure 1
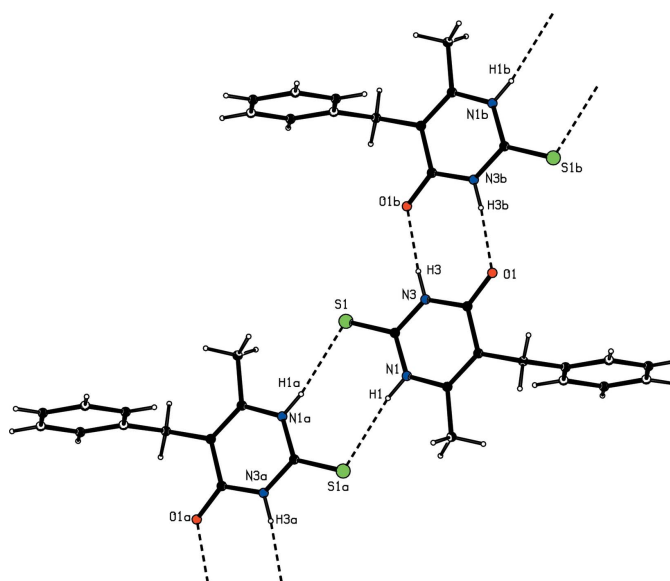A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Figure 2
Part of the N—H···S and N—H···O hydrogen-bonded (dashed lines) chain in (I). [Symmetry codes: (a) $-x, -y, -z+1$; (b) $-x+2, -y, -z+2$.]

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