Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

5-Butyl-6-methyl-2-thioxo-2,3-dihydropyrimidin-4(1*H*)-one

Tao Long,[a] Hong-Bin Zhou[b] and An-Xin Wu[a]*

[a]Key Laboratory of Pesticide and Chemical Biology of Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China, and [b]College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

Correspondence e-mail: chwuax@mail.ccnu.edu.cn

Received 6 June 2005
Accepted 10 June 2005
Online 17 June 2005

In the title compound, $C_9H_{14}N_2OS$, the butyl group is disordered over two orientations. In the crystal structure, the inversion-related molecules are linked by N—H···O [N···O = 2.823 (3) Å] and N—H···S [N···S = 3.346 (2) Å] hydrogen bonds to form chains along [210].

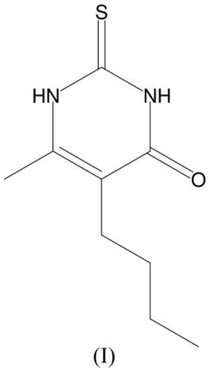
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.057
wR factor = 0.164
Data-to-parameter ratio = 12.0

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

Comment

Pyrimidine derivatives are compounds of considerable biological interest. 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).



(I)

Selected bond lengths and angles in the molecule of (I) are listed in Table 1. As shown in Fig. 1, the *n*-butyl group has two orientations, with C4—C3—C6—C7 and C4—C3—C6—C7′ torsion angles of 114.3 (4) and 72.7 (5)°, respectively. In the crystal structure, inversion-related molecules are linked by N—H···O and N—H···S hydrogen bonds (Table 2) to form chains along [210] (Fig. 2).

Experimental

The title compound was prepared according to the method described by Craig *et al.* (2000) and recrystallized from a solution in acetone by slow evaporation at 283 K.

Crystal data

$C_9H_{14}N_2OS$	$Z = 2$
$M_r = 198.28$	$D_x = 1.277$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo *Kα* radiation
$a = 5.2029$ (14) Å	Cell parameters from 1086 reflections
$b = 7.790$ (2) Å	$\theta = 2.8$–$25.5°$
$c = 13.496$ (4) Å	$\mu = 0.28$ mm^{-1}
$\alpha = 99.166$ (4)°	$T = 292$ (2) K
$\beta = 90.369$ (4)°	Plate, colourless
$\gamma = 106.993$ (4)°	0.30 × 0.20 × 0.08 mm
$V = 515.6$ (2) Å^3	

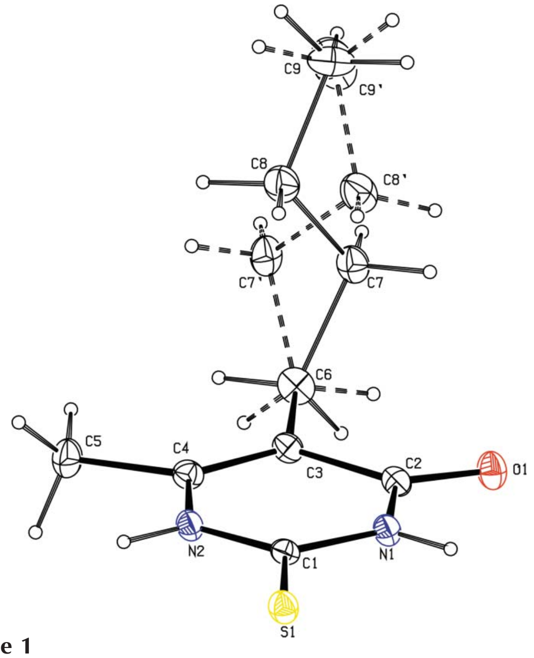


Figure 1
A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Both components of the disordered *n*-butyl chain are shown.

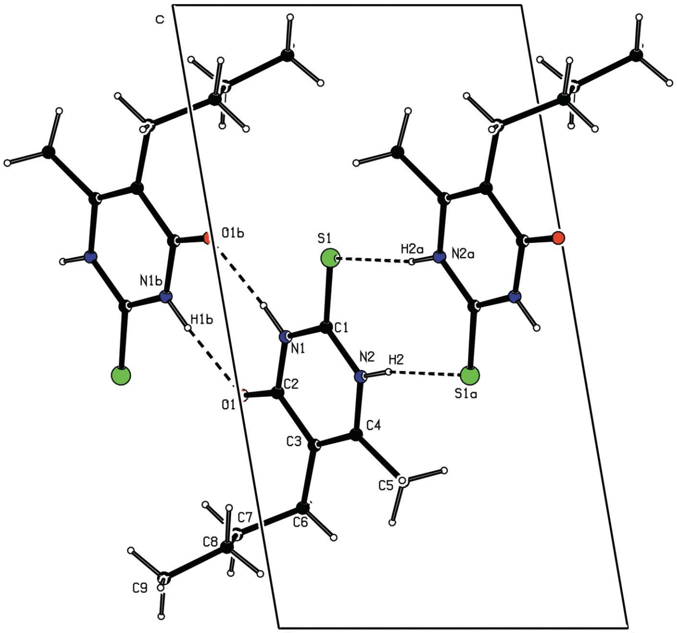


Figure 2
Part of the N—H···S and N—H···O hydrogen bonded (dashed lines) chain in (I). Only one disorder component is shown. [Symmetry codes: (*a*) 2 − *x*, 1 − *y*, 1 − *z* (*b*) −*x*, −*y*, −*z*.]

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
$T_{\min} = 0.921$, $T_{\max} = 0.978$
2885 measured reflections
1793 independent reflections
1416 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.074$
$\theta_{\max} = 25.0°$
$h = -6 \rightarrow 6$
$k = -4 \rightarrow 9$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.165$
$S = 1.06$
1793 reflections
149 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0878P)^2 + 0.0163P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.32$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N2	1.334 (3)	C2—C3	1.458 (4)
C1—N1	1.370 (3)	C3—C4	1.343 (4)
C1—S1	1.668 (3)	C3—C6	1.502 (4)
C2—O1	1.225 (3)	C4—N2	1.360 (4)
C2—N1	1.368 (4)	C4—C5	1.512 (4)
N2—C1—N1	114.4 (3)	C4—C3—C2	117.7 (3)
N2—C1—S1	123.9 (2)	C4—C3—C6	125.0 (3)
O1—C2—C3	123.6 (3)	C3—C4—C5	125.7 (3)
N1—C2—C3	116.3 (2)	N2—C4—C5	113.6 (3)
C6—C7—C8—C9	−175.0 (11)	C6—C7′—C8′—C9′	172.0 (18)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···S1$^{\text{i}}$	0.86	2.49	3.346 (2)	171
N1—H1···O1$^{\text{ii}}$	0.86	1.96	2.823 (3)	176

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

The butyl group was found to be disordered over two orientations. The occupancies of the disordered atoms C7/C7′, C8/C8′ and C9/C9′ were refined to 0.575 (10)/0.425 (10); suitable restraints were applied to the C—C bond lengths. 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 0.95–0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C,N})$ 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*.

The authors are grateful to the Central China Normal University, the National Natural Science Foundation of China (grant No. 20472022) and the Hubei Province Natural Science Fund (grant Nos. 2004ABA085 and 2004ABC002) for financial support.

References

Bruker (1997). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.01. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.

o2170 Long *et al.* • $C_9H_{14}N_2OS$ *Acta Cryst.* (2005). E**61**, o2169–o2171

Craig, G. W., Eberle, M., Lamberth, C. & Vettiger, T. (2000). *J. Prakt. Chem.* **342**, 504–507.

Furberg, S. & Petersen, C. S. (1972). *Acta Chem. Scand.* **26**, 760–768.

Koppel, H. C., Springer, R. H., Robins, R. K. & Cheng, C. C. (1961). *J. Org. Chem.* **26**, 792–803.

Sheldrick, G. M. (1997). *SADABS*, *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Acta Cryst. (2005). E**61**, o2169–o2171 Long *et al.* • $C_9H_{14}N_2OS$ **o2171**