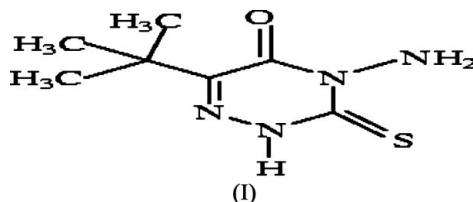


4-Amino-6-*tert*-butyl-3-thioxo-3,4-dihydro-1,2,4-triazin-5(2*H*)-oneB. Sridhar,^a K. Ravikumar,^{a*} H. S. Yathirajan,^b H. G. Anilkumar^b and B. Narayana^c^aLaboratory of X-ray Crystallography, Indian Institute of Chemical Technology, Hyderabad 500 007, India, ^bDepartment of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, and ^cDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, IndiaCorrespondence e-mail:
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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ (C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.115
Data-to-parameter ratio = 14.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.In the title compound, C₇H₁₂N₄OS, the triazine ring is planar. The crystal structure is stabilized by intermolecular N–H···O hydrogen bonds which link the molecules into chains running along the *c* axis.Received 13 February 2006
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Comment

1,2,4-Triazines and the compounds derived from them are found to possess a wide variety of pharmacological activities (Holla *et al.*, 1999). Triazine derivatives include herbicides having a broad spectrum of action that kill many species of weeds, and also herbicides with a narrow selectivity (Gruzdyev *et al.*, 1983). The title compound, (I), is an intermediate in the synthesis of a herbicide, 4-amino-6-(*tert*-butyl)-3-methylthio-1,2,4-triazin-5(4*H*)-one, commonly known as ‘Sencor’ (Eue & Tietz, 1972). It is used for the control of weeds in potato crops and is a broad-spectrum herbicide used in pre-emergence application in potato crops at a rate of 0.75–1 kg per hectare. In view of the importance of the title compound, (I), its crystal structure is reported here.In all essential details, the molecular geometry (Fig. 1 and Table 1) is in good agreement with related structures (Ghassemzadeh *et al.*, 1998). The triazine ring is planar and exists in the thione form; the C=S bond length of 1.663 (2) Å is slightly longer than the pure double-bond distance (1.61 Å; Pauling, 1960). The N–N [1.341 (2) Å] and C–N [mean value 1.341 (2) Å] bond distances are intermediate between the expected single (1.45 and 1.47 Å, respectively) and double (1.20 and 1.27 Å, respectively) bond distances.The crystal structure is stabilized by intra- and intermolecular hydrogen bonds (Table 2). Atom N1 of the triazine ring links the carbonyl O atom of an adjacent triazine ring, forming a chain running parallel to the *c* axis. The tertiary butyl group is oriented such that there are alternate hydrophobic and hydrophilic layers in the crystal packing (Fig. 2).

Experimental

The title compound, (I), was obtained as a gift sample from Rallies India Ltd, Bangalore. The compound was recrystallized by slow evaporation of an acetone–toluene (9:1) solution (m.p. 488 K).

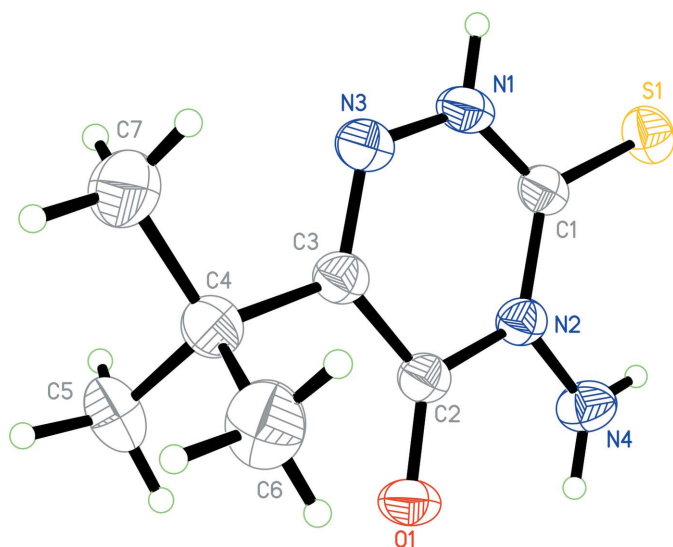


Figure 1

A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

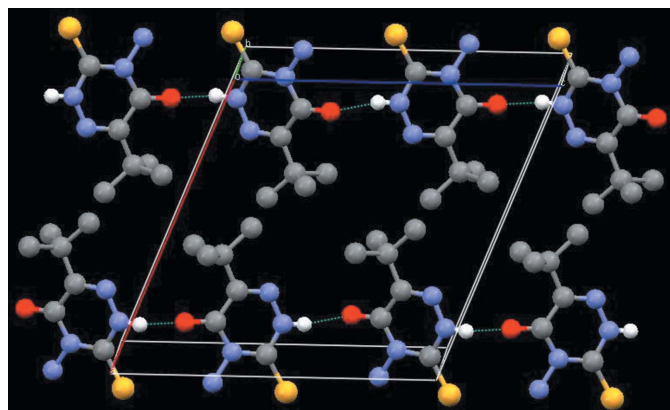


Figure 2

A packing diagram of (I), viewed down the *b* axis, showing the chain formation. Dashed lines indicate N—H...O hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted for clarity.

Crystal data

$C_7H_{12}N_4OS$
 $M_r = 200.27$
 Monoclinic, $P2_1/c$
 $a = 12.5196$ (8) Å
 $b = 6.9535$ (4) Å
 $c = 12.5987$ (8) Å
 $\beta = 112.039$ (1)°
 $V = 1016.64$ (11) Å³
 $Z = 4$

$D_x = 1.308$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 6656 reflections
 $\theta = 3.0$ – 27.9°
 $\mu = 0.29$ mm⁻¹
 $T = 273$ (2) K
 Block, colorless
 $0.21 \times 0.17 \times 0.09$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scan
 Absorption correction: none
 9276 measured reflections
 1780 independent reflections

1640 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.018$
 $\theta_{max} = 25.0^\circ$
 $h = -14 \rightarrow 14$
 $k = -8 \rightarrow 8$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.115$
 $S = 1.07$
 1780 reflections
 121 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0662P)^2 + 0.2933P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.40$ e Å⁻³
 $\Delta\rho_{min} = -0.35$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

C1—N1	1.336 (3)	C2—N2	1.378 (2)
C1—N2	1.370 (2)	C3—N3	1.288 (2)
C2—O1	1.2244 (19)	N2—N4	1.401 (2)
C1—N1—N3	127.70 (15)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...O1 ⁱ	0.86	1.94	2.790 (2)	168
N4—H4B...O1	0.86	2.31	2.607 (2)	100
N4—H4A...S1	0.86	2.59	2.976 (2)	108

Symmetry code: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$.

All H atoms were included in calculated positions ($C-H = 0.93$ – 0.98 Å and $N-H = 0.86$ Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(N,C)$ or $1.5U_{eq}(\text{methyl } C)$. The methyl groups were allowed to rotate but not to tip.

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: *SHELXTL/PC* (Sheldrick, 1990) and *MERCURY* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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