

## 2-Amino-5-propyl-1,3,4-thiadiazole

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## Key indicators

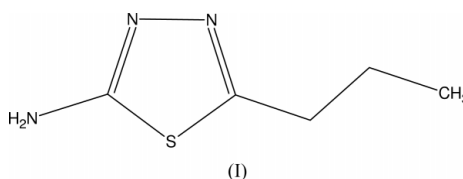
Single-crystal X-ray study  
 T = 293 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.008 \text{ \AA}$   
 R factor = 0.066  
 wR factor = 0.191  
 Data-to-parameter ratio = 16.9

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

The title compound,  $\text{C}_5\text{H}_9\text{N}_3\text{S}$ , which exhibits a hypoglycemic effect, crystallizes in space group  $P2_1/c$ . The structure is held together by a network of intermolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds.

## Comment

The title compound, (I), is an intermediate for the synthesis of 2-toluenesulfonamido-5-propyl-1,3,4-thiadiazole, a compound investigated for its hypoglycemic effect related to its anti-bacterial properties (Matti *et al.*, 1959).



The thiadiazole ring (I) is planar and the propyl group makes an angle of  $49.4 (6)^\circ$  (torsion angle  $\text{S1}-\text{C2}-\text{C3}-\text{C4}$ ) with the plane of the ring. The molecules are linked *via* two different hydrogen bonds, as given in Table 1. These form a hydrogen-bonded network, as shown in Fig. 2.

## Experimental

A mixture of thiasemicarbazide (0.047 mol), butyric acid (0.068 mol) and concentrated sulfuric acid (0.05 mol) was refluxed under anhydrous conditions for 2 h. The reaction mixture was then decomposed by pouring it into ice water. The solution was neutralized with ammonia. The precipitate was collected by filtration and washed with water (Chubb & Nissenbaum, 1959). Yellow crystals (m.p. 476–478 K) were grown from ethanol.

## Crystal data

$\text{C}_5\text{H}_9\text{N}_3\text{S}$   
 $M_r = 143.22$   
 Monoclinic,  $P2_1/c$   
 $a = 10.181 (4) \text{ \AA}$   
 $b = 6.766 (2) \text{ \AA}$   
 $c = 11.114 (4) \text{ \AA}$   
 $\beta = 100.02 (1)^\circ$   
 $V = 753.9 (5) \text{ \AA}^3$   
 $Z = 4$

$D_x = 1.262 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 1701  
 reflections  
 $\theta = 3.5\text{--}24.2^\circ$   
 $\mu = 0.35 \text{ mm}^{-1}$   
 $T = 293 (2) \text{ K}$   
 Prism, yellow  
 $0.35 \times 0.25 \times 0.20 \text{ mm}$

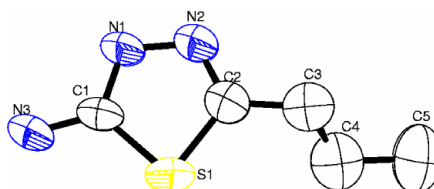


Figure 1

The molecular structure of (I), with ellipsoids at the 50% probability level.

Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: none  
 5894 measured reflections  
 1534 independent reflections

1108 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$   
 $\theta_{\text{max}} = 26.4^\circ$   
 $h = -12 \rightarrow 12$   
 $k = -8 \rightarrow 8$   
 $l = -13 \rightarrow 13$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.066$   
 $wR(F^2) = 0.191$   
 $S = 1.08$   
 1534 reflections  
 91 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1025P)^2 + 0.1974P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.048$   
 $\Delta\rho_{\text{max}} = 0.33 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N3-H1 \cdots N1^i$	0.92	2.06	2.970 (5)	170
$N3-H2 \cdots N2^{ii}$	0.73	2.21	2.944 (4)	176

Symmetry codes: (i)  $-x, 3-y, 1-z$ ; (ii)  $x, \frac{5}{2}-y, z-\frac{1}{2}$ .

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXTL* (Bruker, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3* for Windows (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 1990).

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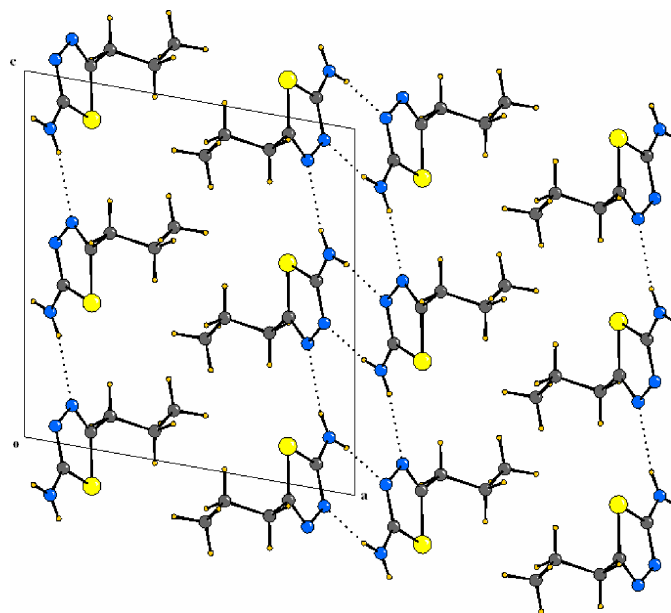


Figure 2

Packing diagram of (I), viewed down the  $b$  axis. Hydrogen bonds are shown as dotted lines.

References

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