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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
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, $C_5H_9N_3S$, which exhibits a hypoglycemic effect, crystallizes in space group $P2_1/c$. The structure is held together by a network of intermolecular N—H···N hydrogen bonds.

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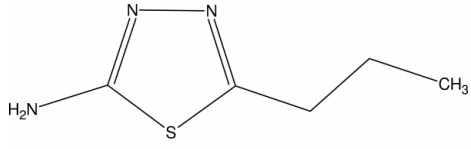
Comment

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 antibacterial properties (Matti *et al.*, 1959).



(I)

The thiadiazole ring (I) is planar and the propyl group makes an angle of 49.4 (6)° (torsion angle S1—C2—C3—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

$C_5H_9N_3S$
M_r = 143.22
Monoclinic, $P2_1/c$
a = 10.181 (4) Å
b = 6.766 (2) Å
c = 11.114 (4) Å
β = 100.02 (1)°
V = 753.9 (5) Å^3
Z = 4
D_x = 1.262 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1701 reflections
θ = 3.5–24.2°
μ = 0.35 mm^{-1}
T = 293 (2) K
Prism, yellow
0.35 × 0.25 × 0.20 mm

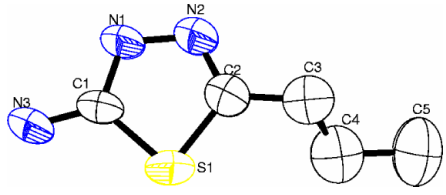


Figure 1
The molecular structure of (I), with ellipsoids at the 50% probability level.

Data collection

Bruker SMART CCD area-detector diffractometer	1108 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.031$
Absorption correction: none	$\theta_{max} = 26.4°$
5894 measured reflections	$h = -12 \rightarrow 12$
1534 independent reflections	$k = -8 \rightarrow 8$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1025P)^2 + 0.1974P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.066$	$(\Delta/\sigma)_{max} = 0.048$
$wR(F^2) = 0.191$	$\Delta\rho_{max} = 0.33$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.17$ e Å^{-3}
1534 reflections	
91 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1···N1^{i}	0.92	2.06	2.970 (5)	170
N3—H2···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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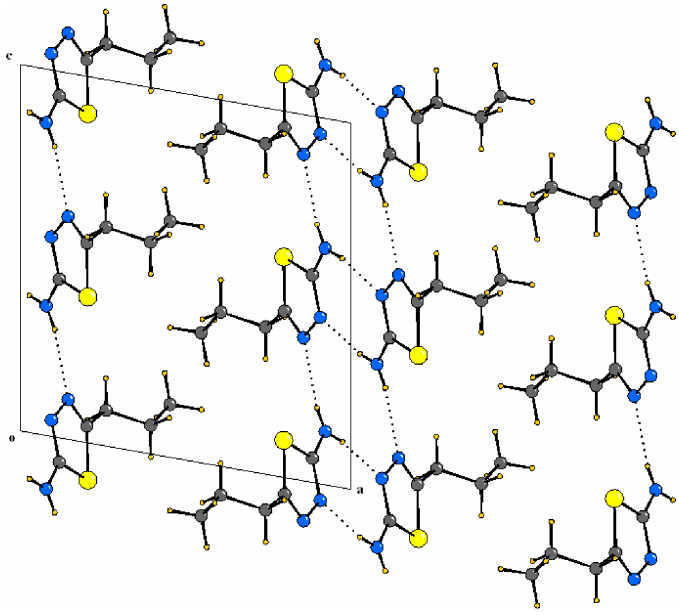

Figure 2
Packing diagram of (I), viewed down the *b* axis. Hydrogen bonds are shown as dotted lines.

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