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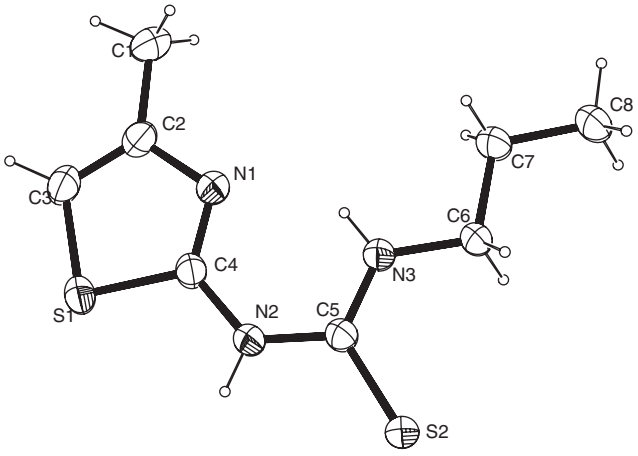
Crystal structure of 1-(4-methylthiazol-2-yl)-3-propylthiourea, $C_8H_{13}N_3S_2$



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Abstract

$C_8H_{13}N_3S_2$, triclinic, $P\bar{1}$ (no. 2), $a = 7.4803(3)$ Å, $b = 8.4562(3)$ Å, $c = 9.3531(3)$ Å, $\alpha = 67.688(1)°$, $\beta = 74.017(1)°$, $\gamma = 85.008(1)°$, $V = 526.07(3)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0256$, $wR_{ref}(F^2) = 0.0736$, $T = 200$ K.

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The crystal structure is shown in the figure. Tables 1–2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Yellow platelets, Size 0.41×0.23×0.18 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ	4.65 cm^{-1}
Diffractometer, scan mode:	Bruker Apex-II CCD, φ and ω scans
$2\theta_{max}$, completeness	56.6°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	18846, 2602, 0.0152
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2399
$N(param)_{refined}$:	128
Programs:	SHELX [3], Bruker programs [4], ShelXle [5] , ORTEP [6], PLATON [7], Mercury [8]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	x	y	z	U_{iso}*/U_{eq}
S1	0.05724(5)	0.78260(3)	0.54364(4)	0.03675(9)
S2	0.10898(4)	0.24429(4)	1.05446(3)	0.03507(9)
N1	0.23601(13)	0.52236(12)	0.50203(11)	0.02899(19)
N2	0.11648(14)	0.49119(12)	0.77548(11)	0.0300(2)
N3	0.25439(13)	0.24054(12)	0.76282(11)	0.02905(19)
C1	0.33401(19)	0.60316(18)	0.20676(14)	0.0409(3)
H1A	0.3203	0.6986	0.1102	0.061*
H1B	0.2780	0.4993	0.2132	0.061*
H1C	0.4664	0.5851	0.2021	0.061*
C2	0.23844(16)	0.64368(14)	0.35123(13)	0.0316(2)
C3	0.15066(18)	0.79027(15)	0.35125(14)	0.0369(3)
H3	0.1417	0.8848	0.2576	0.044*
C4	0.14612(15)	0.57909(13)	0.61266(13)	0.0276(2)
C5	0.16433(14)	0.32642(13)	0.85237(12)	0.0265(2)
C6	0.31288(16)	0.06430(14)	0.82749(13)	0.0310(2)
H6A	0.2048	−0.0090	0.9036	0.037*
H6B	0.4068	0.0578	0.8861	0.037*
C7	0.39489(18)	0.00129(15)	0.69218(13)	0.0351(2)
H7A	0.5030	0.0751	0.6168	0.042*
H7B	0.3010	0.0102	0.6329	0.042*
C8	0.4566(2)	−0.18311(17)	0.75324(16)	0.0437(3)
H8A	0.5079	−0.2196	0.6626	0.066*
H8B	0.3496	−0.2567	0.8270	0.066*
H8C	0.5520	−0.1918	0.8095	0.066*
H2	0.060(2)	0.546(2)	0.833(2)	0.049(4)*
H3A	0.2749(19)	0.2917(18)	0.6643(18)	0.032(3)*

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Source of material

The title compound was prepared by boiling under reflux an equi molar ratio of 2-methyl-4-methylthiazole and propylisothiocyanate for 3 h in ethanol as solvent. The reaction product was filtered off, washed with ethanol and recrystallized with ethanol affording colorless crystals suitable for a crystallographic study.

Experimental details

Carbon-bound H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with U(H) set to 1.2 U_{eq}(C). The H atoms of the methyl groups were allowed to rotate with a fixed angle around the C—C bond to best fit the experimental electron density (HFIX 137 in the SHELX program suite [3]), with U(H) set to 1.5U_{eq}(C). The nitrogen-bound H atoms were located on a difference Fourier map and refined freely.

Discussion

Thioureas are versatile ligands, the hybrid hard nitrogen-soft sulfur donor atom set yielding a multitude of possibilities for coordination to both hard and soft metal centres. Thioureas are able to coordinate as neutral ligands, monoanions or as dianions. An attractive feature of their chemistry is their ease of synthesis, and the ready modification of the substituents at nitrogen and hence their physical and chemical properties. Thiazole derivatives occur as structural unit in biologically active products as vitamin B1, bacitracin, pencillins and in numerous synthetic drugs, fungicides, dyes, and industrial chemicals.

In the asymmetric unit there is one molecule of the title compound. The molecule is essentially planar with rms deviation of 0.0576 through all non-hydrogen atoms. S1 deviates *most* from this plane by 0.115 Å. There is one intramolecular N3—H3A···N1 hydrogen bond of length 2.022(16) Å, which in terms of graph-set analyses [1, 2] can be described by a $S^1_1(6)$ descriptor. There are also intermolecular N2–H2···S2′ interactions of length 2.479(18) Å, which centrosymmetrically connect pairs of molecules (graph set descriptor: $R^2_2(8)$). The shortest π···π interaction is between adjacent thiazole rings with a centroid-to-centroid distance of 3.6688(7) Å with a slippage of 1.336 Å.

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