

## 4-Methylthiazole-5-carbaldehyde

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## Key indicators

Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å  
 $R$  factor = 0.045  
 $wR$  factor = 0.119  
Data-to-parameter ratio = 11.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title compound,  $\text{C}_5\text{H}_5\text{NOS}$ , was synthesized by oxidation of 5-( $\beta$ -hydroxyethyl)-4-methylthiazole, resulting in the breaking of a C—C bond. The non-H atoms of the molecule are almost coplanar. In the crystal structure, no short contacts are observed between symmetry-related molecules.

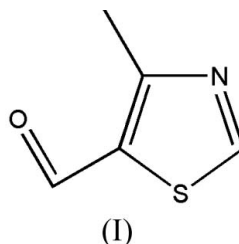
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## Comment

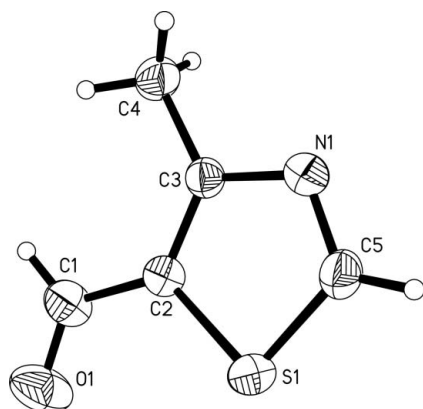
The title compound, (I), is used as a spice, and although its structure is simple there are not many literature references to it. It can be obtained from 4-methylthiazole-5-carbonitrile on reaction with tin(II) dichloride (Harrington & Moggridge, 1939). It can also be prepared from 5-( $\beta$ -hydroxyethyl)-4-methylthiazole with pyridinium dichromate (White & Spencer, 1982), and from *N*-benzenesulfonyl-*N*-(4-methylthiazole-5-carbonyl)hydrazine (Song *et al.*, 2004) as shown by Campaigne *et al.* (1959).



The molecular structure is illustrated in Fig. 1, and selected bond distances and angles are given in Table 1. Atoms C2, C3, C5, N1 and S1 are almost coplanar, forming a five-membered ring with a mean deviation of 0.0047 (4) Å. The O1—C1—C2—S1 torsion angle is 3.9 (6)°, indicating that the aldehyde group is approximately coplanar with the five-membered ring. Similarly, atom C4 deviates from the ring plane by 0.0029 (4) Å. Thus the whole molecule, except for methyl H atoms, is essentially planar, with maximum deviations of 0.0284 Å for atoms C1 and O1. Owing to the presence of the heteroatoms in the five-membered ring, the C3—C2—S1 angle is 110.2 (3)°, deviating from the normal  $sp^2$ -hybridized value. In the crystal structure, there are no significant interactions (intermolecular distances < 3.3 Å) observed between symmetry-related molecules.

## Experimental

The title compound was prepared according to the procedure of White & Spencer (1982). The reaction residue was extracted with diethyl ether. All extracts were filtered by flash chromatography. The filtrate was evaporated to dryness *in vacuo* and sublimed (m.p. 341–343 K). Single crystals suitable for crystallographic analysis were



**Figure 1**  
View of the molecule structure of (I) showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

obtained by slow evaporation of an ethyl-*n*-hexane solution (1:5 v/v).  $^1\text{H NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  10.18 (s, 1H), 9.02 (s, 1H), 2.79 (s, 3H).

#### Crystal data

$\text{C}_5\text{H}_5\text{NOS}$   
 $M_r = 127.17$   
Orthorhombic,  $Pna2_1$   
 $a = 22.574$  (8) Å  
 $b = 3.9269$  (15) Å  
 $c = 6.626$  (2) Å  
 $V = 587.4$  (4) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.438$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
Cell parameters from 1251 reflections  
 $\theta = 3.6$ – $26.1^\circ$   
 $\mu = 0.44$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
Block, colorless  
 $0.22 \times 0.20 \times 0.16$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{\min} = 0.908$ ,  $T_{\max} = 0.932$   
2830 measured reflections

882 independent reflections  
685 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.098$   
 $\theta_{\text{max}} = 26.4^\circ$   
 $h = -28 \rightarrow 28$   
 $k = -4 \rightarrow 4$   
 $l = -4 \rightarrow 8$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.119$   
 $S = 1.16$   
882 reflections  
75 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.23$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983),  
233 Friedel pairs  
Flack parameter: 0.00 (17)

**Table 1**

Selected geometric parameters ( $^\circ$ ).

C3–C2–S1	110.2 (3)
O1–C1–C2–S1	–3.9 (6)

All H atoms were positioned geometrically and refined as riding (C–H = 0.93–0.96 Å). For the CH groups,  $U_{\text{iso}}(\text{H})$  values were set at  $1.2U_{\text{eq}}(\text{carrier atom})$ , and for the methyl groups, they were set at  $1.5U_{\text{eq}}(\text{carrier atom})$ .

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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