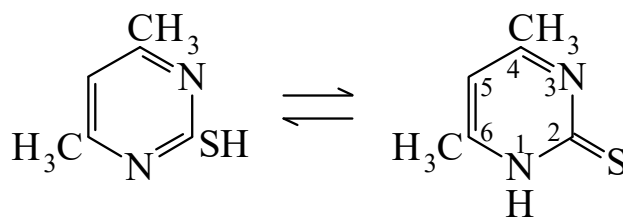




>>Entry Name: **4,6-Dimethyl-2-pyrimidinethiol**

Synonym(s): 4,6-Dimethyl-2(1*H*)-pyrimidinethione, 9CI. 4,6-Dimethyl-2-thio-2,3-dihydropyrimidine. 2-Mercapto-4,6-dimethylpyrimidine. Acetylacetone-thiourea



CAS Registry Number: 22325-27-5

Molecular Formula: C₆H₈N₂S

Molecular Weight: 140.209

Accurate Mass: 140.040818

Percentage Composition: C 51.40%; H 5.75%; N 19.98%; S 22.87%

Source/Synthesis: Condensation prod. of 2,4-Pentanedione [DFS50-O](#) and Thiourea [HGW79-W](#)

Biological Use/Importance: Shows antibacterial and antiviral props.

Physical Description: Light-yellow prisms (EtOH)

Melting Point: Mp 210°

Aldrich: 13801-0

Fluka: 40761

>>**Derivative:** Na salt

CAS Registry Number: 41840-27-1

Physical Description: Cryst. (EtOH)

Melting Point: Mp 300°

>>**Variant:** *NH*-form

Molecular Formula: C₆H₈N₂S

Molecular Weight: 140.209

Accurate Mass: 140.040818

Percentage Composition: C 51.40%; H 5.75%; N 19.98%; S 22.87%

>>**Derivative:** 1-Me

Molecular Formula: C₇H₁₀N₂S

Molecular Weight: 154.235

Accurate Mass: 154.056468

Percentage Composition: C 54.51%; H 6.53%; N 18.16%; S 20.79%

Physical Description: Small needles (C₆H₆)

Melting Point: Mp 156.5°

>>**Variant:** *SH*-form

Molecular Formula: C₆H₈N₂S

Molecular Weight: 140.209

Accurate Mass: 140.040818

Percentage Composition: C 51.40%; H 5.75%; N 19.98%; S 22.87%

>>**Derivative:** *S*-*tert*-Butyloxycarbonyl

see *S*-(4,6-Dimethyl-2-pyrimidinyl)carbonothioic acid, [KJK62-G](#)

References:

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 699C, (*nmr*)

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Hale, W.J. *et al.*, *J.A.C.S.*, 1915, **37**, 594-600, (*synth*)

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Voigt, H. *et al.*, *Z. Chem.*, 1974, **14**, 436, (*Na salt*)

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