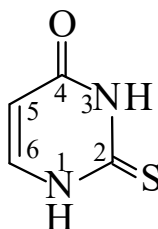




>>Entry Name: **2,3-Dihydro-2-thioxo-4(1*H*)-pyrimidinone**, 9Cl

Synonym(s): 2-Thiouracil. 4-Hydroxy-2-mercaptopyrimidine. Thiouracil. Deracil



CAS Registry Number: 141-90-2

Extra CAS Registry Numbers(s): 156-82-1

Molecular Formula: C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>OS

Molecular Weight: 128.154

Accurate Mass: 128.004433

Percentage Composition: C 37.49%; H 3.15%; N 21.86%; O 12.48%; S 25.02%

General Statement: 6 Tautomers theoretically possible; *NH*-form (illus.) prob. predominates

Biological Source: Present in *E. coli* t-RNA

Use/Importance: Used as 0.3% soln. in Me<sub>2</sub>CO/HCl (pH 1) for photometric detn. of Pd(II) ( $\lambda_{\text{max}}$  428 nm)

Biological Use/Importance: Shows antibacterial and antiviral props. by alterations to protein synth. Formerly used as an antithyroid agent. Antidote for Hg poisoning.

Physical Description: Prisms (H<sub>2</sub>O or EtOH)

Melting Point: Mp 340 dec.°

Solubility: Sol. Me<sub>2</sub>CO, EtOH, H<sub>2</sub>O

Hazard & Toxicity: Exp. carcinogen, human and exp. teratogen. LD<sub>50</sub> (mus, orl) 3900 mg/kg

Aldrich: 11558-4

Fluka: 89060

Sigma: T7750

>>Variant: *NH*-form

Molecular Formula: C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>OS

Molecular Weight: 128.154

Accurate Mass: 128.004433

Percentage Composition: C 37.49%; H 3.15%; N 21.86%; O 12.48%; S 25.02%

>>Derivative: 1-Me

CAS Registry Number: 615-78-1

Molecular Formula: C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>OS

Molecular Weight: 142.181

Accurate Mass: 142.020083

Percentage Composition: C 42.24%; H 4.25%; N 19.70%; O 11.25%; S 22.55%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 226°

>>Derivative: 3-Me

CAS Registry Number: 576-28-3

Molecular Formula: C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>OS

Molecular Weight: 142.181

Accurate Mass: 142.020083

Percentage Composition: C 42.24%; H 4.25%; N 19.70%; O 11.25%; S 22.55%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 207°

>>Derivative: 1,3-Di-Me

Molecular Formula: C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>OS

Molecular Weight: 156.208

Accurate Mass: 156.035733

Percentage Composition: C 46.13%; H 5.16%; N 17.93%; O 10.24%; S 20.53%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 109°