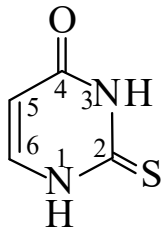
>>**Entry Name: 2,3-Dihydro-2-thioxo-4(1*H*)-pyrimidinone,** 9CI
Synonym(s): 2-Thiouracil. 4-Hydroxy-2-mercaptopyrimidine. Thiouracil. Deracil



CAS Registry Number: 141-90-2
Extra CAS Registry Numbers(s): 156-82-1

Molecular Formula: $C_4H_4N_2OS$
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_2CO/HCl (pH 1) for photometric detn. of Pd(*II*) (λ_{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_2O or EtOH)
Melting Point: Mp 340 dec.°
Solubility: Sol. Me_2CO, EtOH, H_2O
Hazard & Toxicity: Exp. carcinogen, human and exp. teratogen. LD_{50} (mus, orl) 3900 mg/kg

Aldrich: 11558-4
Fluka: 89060
Sigma: T7750

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

Molecular Formula: $C_4H_4N_2OS$
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: $C_5H_6N_2OS$
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: $C_5H_6N_2OS$
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: $C_6H_8N_2OS$
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°