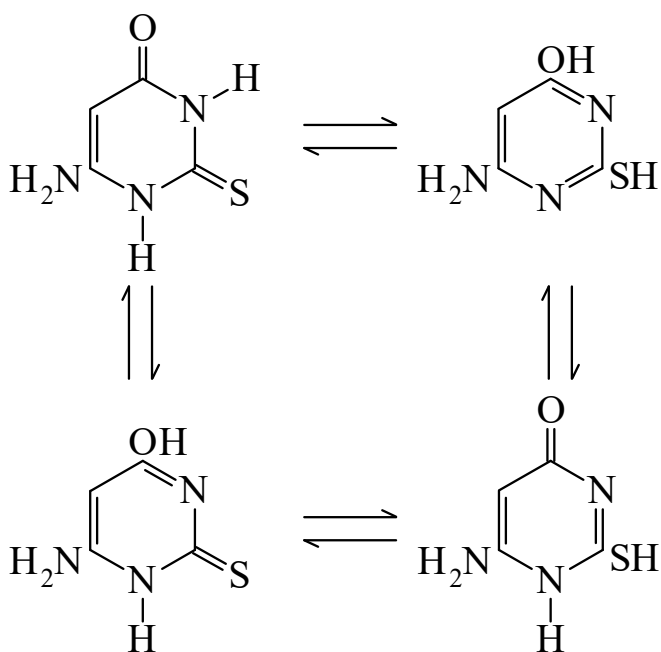




>>Entry Name: 6-Amino-2,3-dihydro-2-thioxo-4(1*H*)-pyrimidinone, 9CI

Synonym(s): 6-Amino-2,5-dihydro-2-thioxo-4(3*H*)-pyrimidinone, 9CI. 4-Amino-6-hydroxy-2-mercaptopyrimidine. 6-Amino-2-thiouracil, 8CI



CAS Registry Number: 1004-40-6

Related CAS Registry Numbers(s): 42985-76-2

Extra CAS Registry Numbers(s): 65802-56-4

Molecular Formula: C₄H₅N₃OS

Molecular Weight: 143.169

Accurate Mass: 143.015332

Percentage Composition: C 33.56%; H 3.52%; N 29.35%; O 11.18%; S 22.40%

General Statement: Other tautomers also possible

Physical Description: Fine needles

Melting Point: Mp 310°

Solubility: V. sol. hot H₂O; insol. Et₂O, C₆H₆

pKa Value: pK_a 7.05 (H₂O)

Sigma: A7879

>>Derivative: O-Me

Synonym(s): 6-Amino-4-methoxy-2(1*H*)-pyrimidinethione, 9CI. 6-Amino-4-methoxy-2-thioxo-1,2-dihydropyrimidine

CAS Registry Number: 66380-54-9

Molecular Formula: C₅H₇N₃OS

Molecular Weight: 157.196

Accurate Mass: 157.030982

Percentage Composition: C 38.20%; H 4.49%; N 26.73%; O 10.18%; S 20.40%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 234-236° (sinters from 219°)

>>Derivative: N¹-Me

Synonym(s): 6-Amino-2,3-dihydro-1-methyl-2-thioxo-4(1*H*)-pyrimidinone, 9CI

CAS Registry Number: 16837-08-4

Molecular Formula: C₅H₇N₃OS

Molecular Weight: 157.196

Accurate Mass: 157.030982

Percentage Composition: C 38.20%; H 4.49%; N 26.73%; O 10.18%; S 20.40%

Physical Description: Needles (H₂O)

Melting Point: Mp 271-272 dec.°