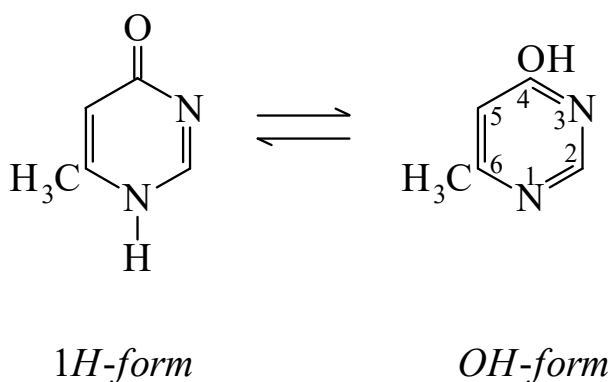




>>Entry Name: 4-Hydroxy-6-methylpyrimidine

Synonym(s): 6-Methyl-4(1*H*)-pyrimidinone. 6-Methyl-4-pyrimidinol. 6-Methyl-4-pyrimidone



CAS Registry Number: 3524-87-6

Molecular Formula: C₅H₆N₂O

Molecular Weight: 110.115

Accurate Mass: 110.048013

Percentage Composition: C 54.54%; H 5.49%; N 25.44%; O 14.53%

Physical Description: Cryst. (Me₂CO, EtOH or EtOAc)

Melting Point: Mp 148-149°

pKa Value: p*K*_{a1} 2.06; p*K*_{a2} 9.1

Hazard & Toxicity: LD₅₀ (mus, ipr) 213 mg/kg

>>Variant: 1*H*-form

Molecular Formula: C₅H₆N₂O

Molecular Weight: 110.115

Accurate Mass: 110.048013

Percentage Composition: C 54.54%; H 5.49%; N 25.44%; O 14.53%

>>Derivative: *N*-Me

Synonym(s): 1,6-Dimethyl-4(1*H*)-pyrimidinone

Molecular Formula: C₆H₈N₂O

Molecular Weight: 124.142

Accurate Mass: 124.063663

Percentage Composition: C 58.05%; H 6.50%; N 22.57%; O 12.89%

Physical Description: Yellow cryst. (2-ethoxyethanol) (as picrate)

Melting Point: Mp 174-176° (picrate)

>>Variant: 3*H*-form

Molecular Formula: C₅H₆N₂O

Molecular Weight: 110.115

Accurate Mass: 110.048013

Percentage Composition: C 54.54%; H 5.49%; N 25.44%; O 14.53%

>>Derivative: *N*-Me

Synonym(s): 3,6-Dimethyl-4(1*H*)-pyrimidinone, 9CI

CAS Registry Number: 17758-19-9

Molecular Formula: C₆H₈N₂O

Molecular Weight: 124.142

Accurate Mass: 124.063663

Percentage Composition: C 58.05%; H 6.50%; N 22.57%; O 12.89%

Physical Description: Prisms (CCl₄)

Melting Point: Mp 80-82°

>>Variant: *OH*-form

Molecular Formula: C₅H₆N₂O

Molecular Weight: 110.115

Accurate Mass: 110.048013

Percentage Composition: C 54.54%; H 5.49%; N 25.44%; O 14.53%