



>>Entry Name: 4-Hydroxy-5-methylpyrimidine

Synonym(s): 5-Methyl-4-pyrimidinol, 9Cl. 5-Methyl-4(3*H*)-pyrimidinone

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. (EtOH/EtOAc)

Melting Point: Mp 153-154°

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: 1-Me

Synonym(s): 1,5-Dimethyl-4(1*H*)-pyrimidinone

CAS Registry Number: 17758-27-9

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: Cryst. (MeOH/EtOAc)

Melting Point: Mp 140-141°

pKa Value: p*K*_a 2.44 (20°)

>>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: 3-Me

Synonym(s): 1,5-Dimethyl-6(1*H*)-pyrimidinone

CAS Registry Number: 17758-26-8

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: Cryst. (EtOAc)

Melting Point: Mp 59°

pKa Value: p*K*_a 2.23 (20°)

Other Data: Hygroscopic

>>Variant: *OH*-form

CAS Registry Number: 17758-52-0

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%