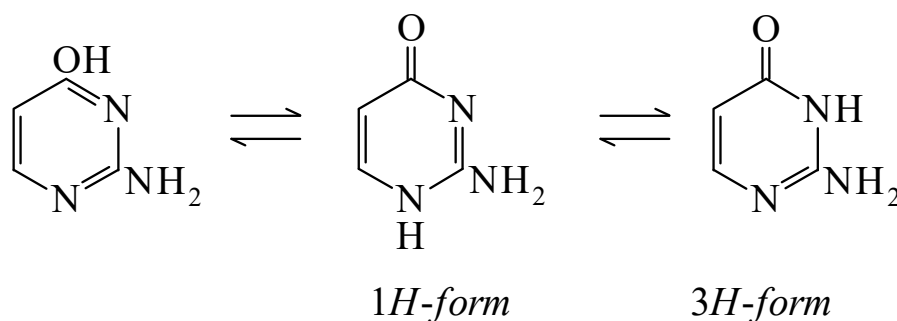




>>Entry Name: 2-Amino-4-hydroxypyrimidine

Synonym(s): 2-Amino-4(1*H*)-pyrimidinone, 9Cl. 2-Amino-4-pyrimidinol. Isocytosine



CAS Registry Number: 108-53-2

Molecular Formula: C₄H₅N₃O

Molecular Weight: 111.103

Accurate Mass: 111.043262

Percentage Composition: C 43.24%; H 4.54%; N 37.82%; O 14.40%

General Statement: *NH*-forms predominate

Physical Description: Prisms (H₂O)

Melting Point: Mp 280 dec.°

pKa Value: p*K*_{a1} 3.91; p*K*_{a2} 9.54 (25°)

Rare Chemicals Library: S36644-7

Sigma: I2127

>>Variant: 1*H*-form

Molecular Formula: C₄H₅N₃O

Molecular Weight: 111.103

Accurate Mass: 111.043262

Percentage Composition: C 43.24%; H 4.54%; N 37.82%; O 14.40%

>>Derivative: 1-Me

CAS Registry Number: 2080-17-3

Molecular Formula: C₅H₇N₃O

Molecular Weight: 125.13

Accurate Mass: 125.058912

Percentage Composition: C 47.99%; H 5.64%; N 33.58%; O 12.79%

Physical Description: Prisms (MeOH)

Melting Point: Mp 276-279 dec.°

>>Derivative: *N*⁺-D-Glucoside

Physical Description: Cryst.

Melting Point: Mp 166 dec.°

Optical Rotation: [α]_D²⁴ -72.6

>>Derivative: *N*⁺-D-Glucoside, tetra-Ac

Physical Description: Cryst.

Melting Point: Mp 131-132°

Optical Rotation: [α]_D¹³ -17.7 (MeOH)

>>Derivative: 1-β-D-Ribopyranosyl

Synonym(s): Isocytidine

CAS Registry Number: 489-59-8

Molecular Formula: C₉H₁₃N₃O₅

Molecular Weight: 243.219

Accurate Mass: 243.085522

Percentage Composition: C 44.45%; H 5.39%; N 17.28%; O 32.89%

Biological Source: Isol. from a strain of *Penicillium brevicompactum*

Physical Description: Glass

Other Data: λ_{max} 256 nm, λ_{min} 240 nm (H₂O, pH1)