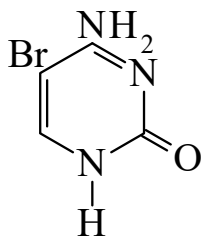




>>Entry Name: 4-Amino-5-bromo-2-hydroxypyrimidine

Synonym(s): 4-Amino-5-bromo-2(1*H*)-pyrimidinone, 9Cl. 5-Bromocytosine, 8Cl



CAS Registry Number: 2240-25-7

Related CAS Registry Numbers(s): 31295-39-3

Molecular Formula: C₄H₄BrN₃O

Molecular Weight: 189.999

Accurate Mass: 188.973773

Percentage Composition: C 25.29%; H 2.12%; Br 42.05%; N 22.12%; O 8.42%

Physical Description: Prisms (H₂O)

Melting Point: Mp 170-171°

Aldrich: 15064-9

Fluka: 16845

Sigma: B4752

>>Derivative: Hydrobromide

CAS Registry Number: 71647-17-1

Physical Description: Cryst.

Melting Point: Mp 255-256 dec.°

>>Derivative: 1-Me

CAS Registry Number: 65567-60-4

Molecular Formula: C₅H₆BrN₃O

Molecular Weight: 204.026

Accurate Mass: 202.989423

Percentage Composition: C 29.43%; H 2.96%; Br 39.16%; N 20.60%; O 7.84%

Physical Description: Yellow cryst. + ½H₂O

Melting Point: Mp 210-215°

pKa Value: pK_a 15.1

>>Derivative: 1,*N*⁴-Di-Me

CAS Registry Number: 71647-19-3

Molecular Formula: C₆H₈BrN₃O

Molecular Weight: 218.053

Accurate Mass: 217.005073

Percentage Composition: C 33.05%; H 3.70%; Br 36.64%; N 19.27%; O 7.34%

Physical Description: Orange cryst. (CHCl₃/petrol)

Melting Point: Mp 175-176°

>>Derivative: 1-β-D-Ribofuranosyl

Synonym(s): 5-Bromocytidine

CAS Registry Number: 3066-86-2

Molecular Formula: C₉H₁₂BrN₃O₅

Molecular Weight: 322.115

Accurate Mass: 321.016033

Percentage Composition: C 33.56%; H 3.75%; Br 24.81%; N 13.05%; O 24.83%

Physical Description: Cryst.

Melting Point: Mp 182-183°

Sigma: B5132