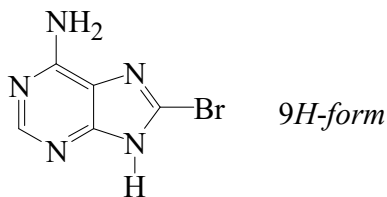




>>Entry Name: 6-Amino-8-bromopurine

Synonym(s): 8-Bromo-1*H*-purin-6-amine, 9Cl. 8-Bromoadenine, 8Cl



CAS Registry Number: 6974-78-3

Molecular Formula: C₅H₄BrN₅

Molecular Weight: 214.024

Accurate Mass: 212.985006

Percentage Composition: C 28.06%; H 1.88%; Br 37.33%; N 32.72%

>>Derivative: 9-β-D-Ribofuranosyl

Synonym(s): 8-Bromoadenosine, 9Cl

CAS Registry Number: 2946-39-6

Molecular Formula: C₁₀H₁₂BrN₅O₄

Molecular Weight: 346.14

Accurate Mass: 345.027266

Percentage Composition: C 34.70%; H 3.49%; Br 23.08%; N 20.23%; O 18.49%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 234° (dec.)

Optical Rotation: $[\alpha]_D^{30} -55$ (c, 2.5 in aq. DMSO)

>>Derivative: 9-β-D-Ribofuranosyl, 2',3',5'-tri-Ac

CAS Registry Number: 31281-86-4

Molecular Formula: C₁₆H₁₈BrN₅O₇

Molecular Weight: 472.252

Accurate Mass: 471.058961

Percentage Composition: C 40.69%; H 3.84%; Br 16.92%; N 14.83%; O 23.72%

Physical Description: Cryst. (THF)

Melting Point: Mp 187-188°

>>Derivative: 9-β-D-Ribofuranosyl, 5'-phosphate

Synonym(s): 8-Bromo-5'-adenylic acid. 8-Bromoadenosine 5'-(dihydrogen phosphate)

CAS Registry Number: 23567-96-6

Molecular Formula: C₁₀H₁₃BrN₅O₇P

Molecular Weight: 426.12

Accurate Mass: 424.993598

Percentage Composition: C 28.19%; H 3.07%; Br 18.75%; N 16.44%; O 26.28%; P 7.27%

Use/Importance: Key intermed. in synth. of 8-substd. purine nucleotides

UV: [neutral] $\lambda_{\max}$ 265 () (no solvent reported)

>>Derivative: 9-β-D-Ribofuranosyl, 5'-triphosphate

Synonym(s): 8-Bromoadenosine 5'-(tetrahydrogen triphosphate). 8-Bromo-ATP

CAS Registry Number: 23567-97-7

Molecular Formula: C₁₀H₁₅BrN₅O₁₃P₃

Molecular Weight: 586.08

Accurate Mass: 584.926262

Percentage Composition: C 20.49%; H 2.58%; Br 13.63%; N 11.95%; O 35.49%; P 15.85%

Other Data: ATP analogue

References: