



Percentage Composition: C 39.74%; H 3.33%; N 46.34%; O 10.59%

Physical Description: Needles

Melting Point: Mp 300°

Other Data: Exists in H₂O as a tautomeric mixt. of oxide and N-OH tautomers. Claimed synthesis of this oxide prior to 1995 appear to be erroneous. The normal oxidn. prod. of adenine is the 1-oxide

>>Derivative: *N*⁹-Oxide

Synonym(s): 9-Hydroxyadenine

CAS Registry Number: 61193-39-3

Molecular Formula: C₅H₅N₅O

Molecular Weight: 151.127

Accurate Mass: 151.04941

Percentage Composition: C 39.74%; H 3.33%; N 46.34%; O 10.59%

Physical Description: Cryst.

Other Data: Tautomeric

>>Derivative: 6*N*-Benzoyl

CAS Registry Number: 4005-49-6

Molecular Formula: C₁₂H₉N₅O

Molecular Weight: 239.236

Accurate Mass: 239.08071

Percentage Composition: C 60.25%; H 3.79%; N 29.27%; O 6.69%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 242-244 dec.°

pKa Value: p*K*_a 2.1 (20°, H₂O)

UV: [neutral] λ_{max} 287 () (0.01*M* HCl aq.)

>>Derivative: 6*N*-Me

Synonym(s): 6-(Methylamino)purine

CAS Registry Number: 443-72-1

Molecular Formula: C₆H₇N₅

Molecular Weight: 149.155

Accurate Mass: 149.070145

Percentage Composition: C 48.32%; H 4.73%; N 46.95%

Biological Source: Minor constit. of bacterial and viral DNA

Melting Point: Mp 312-314 dec.°

pKa Value: p*K*_{a1} 4.18; p*K*_{a2} 9.99 (H₂O)

Fluka: 65700

Sigma: M5376