Percentage Composition: C 39.74%; H 3.33%; N 46.34%; O 10.59%
Physical Description: Hemihydrate
Melting Point: Mp 350 dec.°

>>**Derivative:** N^7-Oxide

CAS Registry Number: 21149-25-7
Molecular Formula: $C_5H_5N_5O$
Molecular Weight: 151.127
Accurate Mass: 151.04941
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 H_2O 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: $C_5H_5N_5O$
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: $C_{12}H_9N_5O$
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: pK_a 2.1 (20°,H_2O)
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: $C_6H_7N_5$
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: pK_{a1} 4.18; pK_{a2} 9.99 (H_2O)
Fluka: 65700
Sigma: M5376

>>**Derivative:** 6*N*-Me, N^1-oxide

CAS Registry Number: 178754-96-6
Molecular Formula: $C_6H_7N_5O$
Molecular Weight: 165.154
Accurate Mass: 165.06506
Percentage Composition: C 43.64%; H 4.27%; N 42.40%; O 9.69%
Physical Description: Needles (H_2O)
Melting Point: Mp 300°