



>>Entry Name: 4-Aminopyrimidine

Synonym(s): 4-Pyrimidinamine, 9CI

CAS Registry Number: 591-54-8

Molecular Formula: C₄H₅N₃

Molecular Weight: 95.104

Accurate Mass: 95.048347

Percentage Composition: C 50.52%; H 5.30%; N 44.18%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 151-152°

pKa Value: pK_a 5.69 (20°)

Aldrich: 26182-3

>>Derivative: 1-Oxide

CAS Registry Number: 84539-20-8

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%

Melting Point: Mp 196-197°

>>Derivative: 4-*N*-Me

Synonym(s): 4-(Methylamino)pyrimidine

CAS Registry Number: 22632-10-6

Molecular Formula: C₅H₇N₃

Molecular Weight: 109.13

Accurate Mass: 109.063997

Percentage Composition: C 55.03%; H 6.47%; N 38.50%

Melting Point: Mp 74-75°

Boiling Point: Bp₁ 142-144°

pKa Value: pK_a 6.09 (23°)

>>Derivative: 4-*N*-Ac

CAS Registry Number: 16166-22-6

Molecular Formula: C₆H₇N₃O

Molecular Weight: 137.141

Accurate Mass: 137.058912

Percentage Composition: C 52.55%; H 5.14%; N 30.64%; O 11.67%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 202°

>>Derivative: 4-*N*-Me; hydrochloride

Physical Description: Needles

>>Derivative: 4-*N*-Me, 1-oxide

CAS Registry Number: 84539-21-9

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%

Melting Point: Mp 137-139.5°