



>>Entry Name: 5-Aminopyrimidine

Synonym(s): 5-Pyrimidinamine, 9CI

CAS Registry Number: 591-55-9

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. (C₆H₆/MeOH)

Melting Point: Mp 170-171°

pKa Value: pK_a 2.51 (25°)

>>Derivative: Methiodide

Physical Description: Yellow-brown cryst.

Melting Point: Mp 166-167°

>>Derivative: *N*-Ac

CAS Registry Number: 45810-14-8

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%

Melting Point: Mp 148-149°

>>Derivative: *N*-Benzoyl

CAS Registry Number: 103854-65-5

Molecular Formula: C₁₁H₉N₃O

Molecular Weight: 199.212

Accurate Mass: 199.074562

Percentage Composition: C 66.32%; H 4.55%; N 21.09%; O 8.03%

Melting Point: Mp 146-147°

>>Derivative: 5-*N*-Me

CAS Registry Number: 40492-24-8

Molecular Formula: C₅H₇N₃

Molecular Weight: 109.13

Accurate Mass: 109.063997

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

Physical Description: Needles

Melting Point: Mp 96.5°

>>Derivative: *N,N*-Di-Me

Synonym(s): *N,N*-Dimethyl-5-pyrimidinamine, 9CI. 5-(Dimethylamino)pyrimidine

CAS Registry Number: 31401-46-4

Molecular Formula: C₆H₉N₃

Molecular Weight: 123.157

Accurate Mass: 123.079647

Percentage Composition: C 58.52%; H 7.37%; N 34.12%

Physical Description: Cryst. by subl.

Melting Point: Mp 79-80°. Mp 172 dec.° (as picrate)

Boiling Point: Bp₁₅ 119°

pKa Value: pK_a 2.96 (25°)

References:

Bowland, M.P.V. *et al.*, *J.C.S.*, 1951, 1218-1221, (*synth*)

Whittaker, N. *et al.*, *J.C.S.*, 1951, 1565-1570, (*synth*)

Girault, G. *et al.*, *Bull. Soc. Chim. Fr.*, 1972, 2787-2798, (*synth, uv*)

Berndt, M. *et al.*, *Chem. Phys. Lett.*, 1973, **19**, 246-250, (*tautom*)

Tsujimoto, T. *et al.*, *Chem. Pharm. Bull.*, 1979, **27**, 691-695, (*pmr, cmr*)

Phillips, O.A. *et al.*, *Can. J. Chem.*, 1999, **77**, 216-222, (*synth, pmr*)