



>>Entry Name: 4,5-Pyrimidinediamine, 9CI

Synonym(s): 4,5-Diaminopyrimidine

CAS Registry Number: 13754-19-3

Molecular Formula: C₄H₆N₄

Molecular Weight: 110.118

Accurate Mass: 110.059246

Percentage Composition: C 43.63%; H 5.49%; N 50.88%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 205-206°

pKa Value: pK_{a1} 6.04; pK_{a2} -0.97 (20°)

Aldrich: D2450-1

Fluka: 33340

Sigma: D2252

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 382A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 823D, (*ir*)

Beaman, A.G. *et al.*, *J.O.C.*, 1962, **27**, 986, (*synth*)

Biffin, M.E.C. *et al.*, *Aust. J. Chem.*, 1967, **20**, 1041, (*synth, pmr*)