



>>Entry Name: 2,4-Diamino-6-chloropyrimidine, 8Cl

Synonym(s): 6-Chloro-2,4-pyrimidinediamine, 9Cl

CAS Registry Number: 156-83-2

Molecular Formula: C₄H₅ClN₄

Molecular Weight: 144.563

Accurate Mass: 144.020273

Percentage Composition: C 33.23%; H 3.49%; Cl 24.52%; N 38.76%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 200-201°

pKa Value: pK_a 3.57

Hazard & Toxicity: Irritant

Aldrich: C3320-4

Fluka: 24250

>>Derivative: 3-Oxide

CAS Registry Number: 35139-67-4

Molecular Formula: C₄H₅ClN₄O

Molecular Weight: 160.562

Accurate Mass: 160.015188

Percentage Composition: C 29.92%; H 3.14%; Cl 22.08%; N 34.89%; O 9.96%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 190 dec.°

pKa Value: pK_a 2.25

Aldrich: 36423-1

>>Derivative: 2,4-*N*-Di-Ph

Molecular Formula: C₁₆H₁₃ClN₄

Molecular Weight: 296.758

Accurate Mass: 296.082873

Percentage Composition: C 64.76%; H 4.42%; Cl 11.95%; N 18.88%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 107-109°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 824D, (*ir*)

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **3**, 484B, (*nmr*)

Aldrich Library of IR Spectra, 1363A, (*ir*)

Hull, R. *et al.*, *J.C.S.*, 1947, 41, (*synth*)

Roth, B. *et al.*, *J.O.C.*, 1969, **34**, 821, (*uv*)

Delia, T.J. *et al.*, *J. Het. Chem.*, 1972, **9**, 73, (*oxide, synth, pmr, uv*)

Staedeli, W. *et al.*, *Helv. Chim. Acta*, 1980, **63**, 504, (*N-15 nmr*)

Cowden, W.B. *et al.*, *Aust. J. Chem.*, 1984, **37**, 1195, (*props, oxide, synth, pmr, uv*)

Schomaker, J.M. *et al.*, *J. Het. Chem.*, 2000, **37**, 1457-1462, (*2,4-N-di-Ph*)