



>>Entry Name: 5-Chloropyrimidine, 9CI

CAS Registry Number: 17180-94-8

Structure by analogy with 2-Chloropyrimidine, [FVV68-S](#)

Molecular Formula: C₄H₃ClN₂

Molecular Weight: 114.534

Accurate Mass: 113.998475

Percentage Composition: C 41.95%; H 2.64%; Cl 30.95%; N 24.46%

Melting Point: Mp 36.5°

>>Derivative: *N*-Oxide

CAS Registry Number: 114969-48-1

Molecular Formula: C₄H₃ClN₂O

Molecular Weight: 130.533

Accurate Mass: 129.99339

Percentage Composition: C 36.81%; H 2.32%; Cl 27.16%; N 21.46%; O 12.26%

Melting Point: Mp 155-156°

References:

Lythgoe, B. *et al.*, *J.C.S.*, 1951, 2323

Kress, T.J. *et al.*, *J. Het. Chem.*, 1983, **20**, 1721, (*synth, ir, uv, pmr, cmr*)

Yamanaka, H. *et al.*, *Chem. Pharm. Bull.*, 1987, **35**, 3119, (*synth, pmr, oxide*)

Ikari, Y. *et al.*, *Bull. Chem. Soc. Jpn.*, 1990, **63**, 2891, (*ir, Raman*)