>>**Entry Name: 6-Chloro-4-pyrimidinecarboxylic acid,** 9Cl

CAS Registry Number: 37131-91-2
Structure by analogy with 2-Chloro-4-pyrimidinecarboxylic acid, BCN33-V

Molecular Formula: $C_5H_3ClN_2O_2$
Molecular Weight: 158.544
Accurate Mass: 157.988305
Percentage Composition: C 37.88%; H 1.91%; Cl 22.36%; N 17.67%; O 20.18%
Physical Description: Yellow cryst. (petrol)
Melting Point: Mp 132-133°
Experimental Log P Data: Log P 2.8 (exp)

>>**Derivative:** Me ester

Molecular Formula: $C_6H_5ClN_2O_2$
Molecular Weight: 172.57
Accurate Mass: 172.003955
Percentage Composition: C 41.76%; H 2.92%; Cl 20.54%; N 16.23%; O 18.54%
Physical Description: Cryst. (petrol)
Melting Point: Mp 60-61°

>>**Derivative:** Amide

Molecular Formula: $C_5H_4ClN_3O$
Molecular Weight: 157.559
Accurate Mass: 157.004289
Percentage Composition: C 38.12%; H 2.56%; Cl 22.50%; N 26.67%; O 10.15%
Physical Description: Cryst. (EtOH)
Melting Point: Mp 162-163°

References:

Daves, G.D. *et al.*, *J. Het. Chem.*, 1964, **1**, 130, *(deriv, uv)*
Cherkasov, V.M. *et al.*, *Khim. Geterotsikl. Soedin.*, 1972, 558; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1972, 509, ***(synth)***
Titov, E.U. *et al.*, *Khim. Geterotsikl. Soedin.*, 1972, 833; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1972, 754, *(synth, ir)*