



>>Entry Name: 4-Chloro-5-pyrimidinecarboxylic acid, 9Cl

Structure by analogy with 2-Chloro-4-pyrimidinecarboxylic acid, [BCN33-V](#)

Molecular Formula: C₅H₃ClN₂O₂

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%

>>Derivative: Et ester

CAS Registry Number: 41103-17-7

Molecular Formula: C₇H₇ClN₂O₂

Molecular Weight: 186.597

Accurate Mass: 186.019605

Percentage Composition: C 45.06%; H 3.78%; Cl 19.00%; N 15.01%; O 17.15%

Boiling Point: Bp_{0.05} 74-75°

>>Derivative: Nitrile

Synonym(s): 4-Chloro-5-cyanopyrimidine

CAS Registry Number: 16357-68-9

Molecular Formula: C₅H₂ClN₃

Molecular Weight: 139.544

Accurate Mass: 138.993724

Percentage Composition: C 43.04%; H 1.44%; Cl 25.41%; N 30.11%

Physical Description: Cryst. (petrol)

Melting Point: Mp 45-47°

References:

Bredereck, H. *et al.*, *Chem. Ber.*, 1962, **95**, 803-809; 1967, **100**, 3664-3670, (*Et ester, nitrile*)

Hermann, K. *et al.*, *Annalen*, 1981, 333-341, (*Et ester*)