



>>Entry Name: 3-Chloro-4-pyridinecarboxylic acid, 9Cl

Synonym(s): 3-Chloroisonicotinic acid, 8Cl

CAS Registry Number: 88912-27-0

Structure by analogy with 2-Chloro-3-pyridinecarboxylic acid, [FVV54-L](#)

Molecular Formula: C₆H₄ClNO₂

Molecular Weight: 157.556

Accurate Mass: 156.993056

Percentage Composition: C 45.74%; H 2.56%; Cl 22.50%; N 8.89%; O 20.31%

Melting Point: Mp 228-230°

Solubility: Sol. EtOH, conc. HCl, spar. sol. hot H₂O

>>Derivative: Me ester

Molecular Formula: C₇H₆ClNO₂

Molecular Weight: 171.583

Accurate Mass: 171.008706

Percentage Composition: C 49.00%; H 3.52%; Cl 20.66%; N 8.16%; O 18.65%

Physical Description: Needles (MeOH)

Melting Point: Mp 32°

Boiling Point: Bp₆ 122-127°

>>Derivative: Nitrile

Synonym(s): 3-Chloro-4-cyanopyridine. 3-Chloroisonicotinonitrile

CAS Registry Number: 68325-15-5

Molecular Formula: C₆H₃ClN₂

Molecular Weight: 138.556

Accurate Mass: 137.998475

Percentage Composition: C 52.01%; H 2.18%; Cl 25.59%; N 20.22%

Physical Description: Solid (petrol)

Melting Point: Mp 71-72°

>>Derivative: Nitrile, N-oxide

Molecular Formula: C₆H₃ClN₂O

Molecular Weight: 154.555

Accurate Mass: 153.99339

Percentage Composition: C 46.63%; H 1.96%; Cl 22.94%; N 18.13%; O 10.35%

Physical Description: Cryst. (toluene)

Melting Point: Mp 176-179°

>>Derivative: Amide

Molecular Formula: C₆H₅ClN₂O

Molecular Weight: 156.571

Accurate Mass: 156.00904

Percentage Composition: C 46.03%; H 3.22%; Cl 22.64%; N 17.89%; O 10.22%

Physical Description: Yellow cryst.

Melting Point: Mp 165-168°

References:

Meyer, A. *et al.*, *Ber.*, 1928, **61**, 2202-2215, (*synth*)

Fox, H.H. *et al.*, *J.O.C.*, 1958, **23**, 64-66, (*synth, amide*)

Rokach, J. *et al.*, *J. Het. Chem.*, 1978, 683, (*nitrile*)

Krapcho, A.P. *et al.*, *J. Het. Chem.*, 1997, **34**, 27, (*synth, pmr*)

Epsztajn, J. *et al.*, *Synth. Commun.*, 1997, **27**, 1075-1086, (*Me ester*)

Leroy, F. *et al.*, *Synth. Commun.*, 1997, **27**, 2905-2916, (*nitrile*)