



>>Entry Name: 2-Chloro-4-pyridinecarboxylic acid, 9Cl

Synonym(s): 2-Chloroisonicotinic acid, 8Cl

CAS Registry Number: 6313-54-8

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 234-235°

pKa Value: pK_{a1} 2.7

>>Derivative: Me ester

CAS Registry Number: 58481-11-1

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: Oil, cryst. on standing

Boiling Point: Bp₁₅ 84-88°. Bp_{0.05} 52-56°

>>Derivative: Et ester

CAS Registry Number: 54453-93-9

Molecular Formula: C₈H₈ClNO₂

Molecular Weight: 185.609

Accurate Mass: 185.024356

Percentage Composition: C 51.77%; H 4.34%; Cl 19.10%; N 7.55%; O 17.24%

Boiling Point: Bp₂₀ 130-132°

>>Derivative: Chloride

CAS Registry Number: 65287-34-5

Molecular Formula: C₆H₃Cl₂NO

Molecular Weight: 176.001

Accurate Mass: 174.959168

Percentage Composition: C 40.95%; H 1.72%; Cl 40.29%; N 7.96%; O 9.09%

Boiling Point: Bp₁₀ 101°

>>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%

Use/Importance: Commercially available

Physical Description: Fine needles (MeOH)

Melting Point: Mp 201-203°

References:

Büchi, J. *et al.*, *Helv. Chim. Acta*, 1947, **30**, 507-519, (*synth*)

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

Brown, E.V. *et al.*, *J. Het. Chem.*, 1971, **8**, 189-192, (*ms*)

Seydel, J.K. *et al.*, *J. Med. Chem.*, 1976, **19**, 483-492, (*synth*)

Adger, B.M. *et al.*, *J.C.S. Perkin I*, 1988, 2785-2789, (*ester, synth, ir, pmr*)

Anderson, W.K. *et al.*, *J. Med. Chem.*, 1990, **33**, 1667-1675, (*synth, chloride, pmr*)