



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

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

CAS Registry Number: 59290-82-3

Molecular Formula: C₆H₄N₂O₄

Molecular Weight: 168.109

Accurate Mass: 168.017108

Percentage Composition: C 42.87%; H 2.40%; N 16.66%; O 38.07%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 222 dec.°

>>Derivative: Me ester

CAS Registry Number: 103698-10-8

Molecular Formula: C₇H₆N₂O₄

Molecular Weight: 182.135

Accurate Mass: 182.032758

Percentage Composition: C 46.16%; H 3.32%; N 15.38%; O 35.14%

Physical Description: Yellow oil

Boiling Point: Bp₁₀ 140.5-142°

>>Derivative: Amide

CAS Registry Number: 59290-91-4

Molecular Formula: C₆H₅N₃O₃

Molecular Weight: 167.124

Accurate Mass: 167.033092

Percentage Composition: C 43.12%; H 3.02%; N 25.14%; O 28.72%

Physical Description: Needles (H₂O)

Melting Point: Mp 166.5-168°

>>Derivative: Nitrile

Synonym(s): 3-Nitro-4-cyanopyridine

CAS Registry Number: 103698-09-5

Molecular Formula: C₆H₃N₃O₂

Molecular Weight: 149.109

Accurate Mass: 149.022527

Percentage Composition: C 48.33%; H 2.03%; N 28.18%; O 21.46%

Physical Description: Yellow oil which solidifies

Melting Point: Mp 39.5-41°

References:

Brown, E.V., *J.A.C.S.*, 1954, **76**, 3167-3168, (*synth*)

Charton, M. *et al.*, *Chem. Scr.*, 1985, **25**, 340-344, (*amide, nitrile*)

Bakke, J.M. *et al.*, *J. Het. Chem.*, 2001, **38**, 99-104, (*amide*)