



>>Entry Name: 3-Iodo-4-pyridinecarboxylic acid, 9CI

Synonym(s): 3-Iodoisonicotinic acid

CAS Registry Number: 57842-10-1

Molecular Formula: C<sub>6</sub>H<sub>4</sub>INO<sub>2</sub>

Molecular Weight: 249.008

Accurate Mass: 248.928677

Percentage Composition: C 28.94%; H 1.62%; I 50.96%; N 5.63%; O 12.85%

Physical Description: Cryst. (EtOH or MeOH)

Melting Point: Mp 244-244.5° (226°)

>>Derivative: Me ester

CAS Registry Number: 188677-49-8

Molecular Formula: C<sub>7</sub>H<sub>6</sub>INO<sub>2</sub>

Molecular Weight: 263.034

Accurate Mass: 262.944327

Percentage Composition: C 31.96%; H 2.30%; I 48.25%; N 5.33%; O 12.17%

Melting Point: Mp 41-42°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-3-iodopyridine. 3-Iodonicotinonitrile

CAS Registry Number: 10386-28-4

Molecular Formula: C<sub>6</sub>H<sub>3</sub>IN

Molecular Weight: 216.001

Accurate Mass: 215.931022

Percentage Composition: C 33.36%; H 1.40%; I 58.75%; N 6.48%

Physical Description: Yellow cryst. (C<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 111-112°

#### References:

Bachman, G.B. *et al.*, *J.O.C.*, 1949, **14**, 97-104, (*synth*)

Plazek, E. *et al.*, *Rocz. Chem.*, 1952, **26**, 106-109; *CA*, **47**, 7497g, (*synth*)

Talik, T., *Rocz. Chem.*, 1962, **36**, 1049-1056; *CA*, **59**, 7480g, (*nitrile*)

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