



>>Entry Name: 5-Iodo-3-pyridinecarboxylic acid, 9CI

Synonym(s): 5-Iodonicotinic acid

CAS Registry Number: 15366-65-1

Molecular Formula: C₆H₄INO₂

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: Needles (H₂O)

Melting Point: Mp 220°

>>Derivative: Me ester

Molecular Formula: C₇H₆INO₂

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%

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 121°

>>Derivative: Et ester

CAS Registry Number: 63473-00-7

Molecular Formula: C₈H₈INO₂

Molecular Weight: 277.061

Accurate Mass: 276.959977

Percentage Composition: C 34.68%; H 2.91%; I 45.80%; N 5.06%; O 11.55%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 86-87°

>>Derivative: Amide

Synonym(s): 5-Iodonicotinamide, 8CI

CAS Registry Number: 33556-84-2

Molecular Formula: C₆H₅IN₂O

Molecular Weight: 248.023

Accurate Mass: 247.944661

Percentage Composition: C 29.06%; H 2.03%; I 51.17%; N 11.29%; O 6.45%

Physical Description: Leaflets (H₂O)

Melting Point: Mp 221-222°

References:

Graf, R., *J. Prakt. Chem.*, 1933, **138**, 244-258, (*synth, esters, amide*)

Lavilla, R. *et al.*, *Eur. J. Org. Chem.*, 1999, 373-378, (*synth, pmr*)