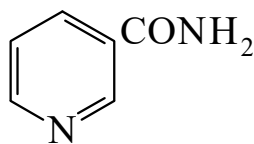




>>Entry Name: 3-Pyridinecarboxamide, 9CI

ENTRY UNDER REVIEW

Synonym(s): Nicotinamide, 8CI, INN. Nicotinic acid amide. Vitamin B₃. Niacinamide. PP-Factor. Antipellagra factor. Many other names



CAS Registry Number: 98-92-0

Related CAS Registry Numbers(s): 6485-44-5

Molecular Formula: C₆H₆N₂O

Molecular Weight: 122.126

Accurate Mass: 122.048013

Percentage Composition: C 59.01%; H 4.95%; N 22.94%; O 13.10%

Biological Source: Widespread in plants, e.g. rice, yeast and fungi

Biological Use/Importance: Enzyme cofactor, used in treatment of pellagra, low mammalian toxicity

Physical Description: Needles (C₆H₆)

Melting Point: Mp 129-130°

Boiling Point: Bp_{0.0005} 150-160°

pKa Value: pK_a 3.33 (20°)

Calculated Log P Data: Log P -0.21 (calc)

Aldrich: N755-9

Fluka: 72340

Sigma: N3768

Supelco: R47-5075

>>Derivative: 1-Oxide

CAS Registry Number: 1986-81-8

Molecular Formula: C₆H₆N₂O₂

Molecular Weight: 138.126

Accurate Mass: 138.042928

Percentage Composition: C 52.17%; H 4.38%; N 20.28%; O 23.17%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 291-293° (285-286°)

Aldrich: N760-5

Sigma: N3258

>>Derivative: 1-Me

>>Derivative: 1-Benzyl

Synonym(s): 1-Benzyl-3-carbamoylpyridinim(1+)

CAS Registry Number: 5096-13-9

Extra CAS Registry Numbers(s): 13076-43-2 16183-83-8

Molecular Formula: C₁₃H₁₃N₂O⁽⁺⁾

Molecular Weight: 213.259

Accurate Mass: 213.102788

Percentage Composition: C 73.22%; H 6.14%; N 13.14%; O 7.50%

Biological Use/Importance: Inhibitor of yeast alcohol dehydrogenase

Physical Description: Cryst. (EtOH/Et₂O) (as chloride)

Melting Point: Mp 236 dec.° (chloride)

>>Derivative: N'-Me

Synonym(s): N-Methyl-3-pyridinecarboxamide, 9CI. N-Methylnicotinamide, 8CI. 3-(Methylcarbamoyl)pyridine

CAS Registry Number: 114-33-0

Molecular Formula: C₇H₈N₂O

Molecular Weight: 136.153

Accurate Mass: 136.063663

Percentage Composition: C 61.75%; H 5.92%; N 20.57%; O 11.75%

Biological Source: Metabolised from Tryptophan [CHP14-U](#) and 3-Pyridinecarboxylic acid [BPB04-S](#); principal urinary excretion product of 3-Pyridinecarboxylic acid [BPB04-S](#) in man, dogs, pigs, rats, etc.