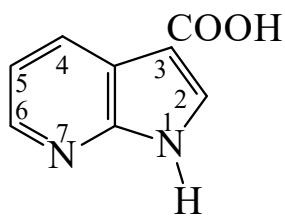




>>Entry Name: 1*H*-Pyrrolo[2,3-*b*]pyridine-3-carboxylic acid, 9CI



CAS Registry Number: 156270-06-3

Molecular Formula: C₈H₆N₂O₂

Molecular Weight: 162.148

Accurate Mass: 162.042928

Percentage Composition: C 59.26%; H 3.73%; N 17.28%; O 19.73%

Physical Description: Cryst.

Melting Point: Mp 235 dec.°

>>Derivative: Et ester

Molecular Formula: C₁₀H₁₀N₂O₂

Molecular Weight: 190.201

Accurate Mass: 190.074228

Percentage Composition: C 63.15%; H 5.30%; N 14.73%; O 16.82%

Physical Description: Needles (C₆H₆/cyclohexane)

Melting Point: Mp 163-164°

>>Derivative: Amide

CAS Registry Number: 74420-16-9

Molecular Formula: C₈H₇N₃O

Molecular Weight: 161.163

Accurate Mass: 161.058912

Percentage Composition: C 59.62%; H 4.38%; N 26.07%; O 9.93%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 275-276 dec.°

>>Derivative: Nitrile

Synonym(s): 3-Cyano-1*H*-pyrrolo[2,3-*b*]pyridine

CAS Registry Number: 4414-89-5

Molecular Formula: C₈H₅N₃

Molecular Weight: 143.148

Accurate Mass: 143.048347

Percentage Composition: C 67.13%; H 3.52%; N 29.35%

Physical Description: Needles (H₂O)

Melting Point: Mp 262-265°

>>Derivative: *N*¹-Me

Synonym(s): 1-Methyl-1*H*-pyrrolo[2,3-*b*]pyridine-3-carboxylic acid

Molecular Formula: C₉H₈N₂O₂

Molecular Weight: 176.174

Accurate Mass: 176.058578

Percentage Composition: C 61.36%; H 4.58%; N 15.90%; O 18.16%

Melting Point: Mp 260°

>>Derivative: *N*¹-Et

Synonym(s): 1-Ethyl-1*H*-pyrrolo[2,3-*b*]pyridine-3-carboxylic acid

CAS Registry Number: 141650-53-5

Molecular Formula: C₁₀H₁₀N₂O₂

Molecular Weight: 190.201

Accurate Mass: 190.074228

Percentage Composition: C 63.15%; H 5.30%; N 14.73%; O 16.82%

Melting Point: Mp 209-210°