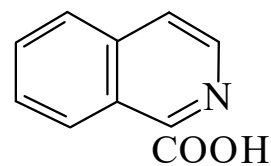




>>Entry Name: 1-Isoquinolinecarboxylic acid

Synonym(s): Isoquinaldinic acid. Isoquinaldic acid



CAS Registry Number: 486-73-7

Molecular Formula: C₁₀H₇NO₂

Molecular Weight: 173.171

Accurate Mass: 173.047679

Percentage Composition: C 69.36%; H 4.07%; N 8.09%; O 18.48%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 161 dec.°

pKa Value: pK_a 4.97 (20°, 0.5M NaCl)

Aldrich: 15013-4

Fluka: 58752

>>Derivative: Me ester

CAS Registry Number: 27104-72-9

Molecular Formula: C₁₁H₉NO₂

Molecular Weight: 187.198

Accurate Mass: 187.063329

Percentage Composition: C 70.58%; H 4.85%; N 7.48%; O 17.09%

Physical Description: Oil

Boiling Point: Bp_{0.1} 114-116°

>>Derivative: Me ester, picrate

CAS Registry Number: 30236-91-0

Melting Point: Mp 147°

>>Derivative: Et ester

CAS Registry Number: 50458-78-1

Molecular Formula: C₁₂H₁₁NO₂

Molecular Weight: 201.224

Accurate Mass: 201.078979

Percentage Composition: C 71.63%; H 5.51%; N 6.96%; O 15.90%

Boiling Point: Bp₂₀ 197-199°

>>Derivative: Et ester, picrate

Physical Description: Cryst. (EtOH)

Melting Point: Mp 129-130°

>>Derivative: Amide

CAS Registry Number: 1436-44-8

Molecular Formula: C₁₀H₈N₂O

Molecular Weight: 172.186

Accurate Mass: 172.063663

Percentage Composition: C 69.76%; H 4.68%; N 16.27%; O 9.29%

Physical Description: Cryst.

Melting Point: Mp 168-170°

>>Derivative: Nitrile

Synonym(s): 1-Cyanoisoquinoline. Isoquinaldinic nitrile