



>>Entry Name: 3-Isoquinolinecarboxylic acid

CAS Registry Number: 6624-49-3

Related CAS Registry Numbers(s): 50458-79-2

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. (H₂O)

Melting Point: Mp 171° (167-168°)

>>Derivative: Me ester

CAS Registry Number: 27104-73-0

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%

Melting Point: Mp 88-89° (86-88°)

Aldrich: 33855-9

>>Derivative: Amide

CAS Registry Number: 50458-77-0

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. (MeOH aq.)

Melting Point: Mp 213° (205-206°)

>>Derivative: Nitrile

Synonym(s): 3-Cyanoisoquinoline

CAS Registry Number: 26947-41-1

Molecular Formula: C₁₀H₆N₂

Molecular Weight: 154.171

Accurate Mass: 154.053098

Percentage Composition: C 77.91%; H 3.92%; N 18.17%

Melting Point: Mp 124-125°

Aldrich: 33853-2

>>Derivative: N-Oxide

Molecular Formula: C₁₀H₇NO₃

Molecular Weight: 189.17

Accurate Mass: 189.042594

Percentage Composition: C 63.49%; H 3.73%; N 7.40%; O 25.37%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 211-211.5°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 460C; 461B, (*nmr*)

Jerchel, D. *et al.*, *Annalen*, 1958, **613**, 153, (*synth*)

Baumgarten, H.E. *et al.*, *J.O.C.*, 1958, **23**, 900, (*synth*)

Hickey, D.M.B. *et al.*, *J.C.S. Perkin 1*, 1987, 921, (*ester*)

Langry, K.C., *Org. Prep. Proced. Int.*, 1994, **26**, 429, (*synth, derivs*)