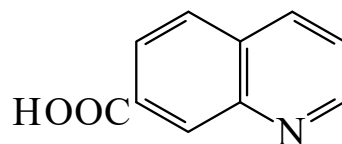




>>Entry Name: 7-Quinolinecarboxylic acid, 9CI



CAS Registry Number: 1078-30-4

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%

Use/Importance: Insecticide

Physical Description: Needles (H₂O or EtOH)

Melting Point: Mp 249-250 subl.°

Solubility: Insol. Et₂O, sol. hot, insol. cold H₂O

pKa Value: pK_a 4.97 (25°, 50% MeOH aq.)

Calculated Log P Data: Log P 2.08 (calc)

>>Derivative: Me ester

CAS Registry Number: 51552-68-2

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 73-76°

>>Derivative: Et ester

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%

Melting Point: Mp 52-53°

Boiling Point: Bp₂ 145-150°

>>Derivative: Amide

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%

Melting Point: Mp 178-179°

>>Derivative: Nitrile

Synonym(s): 7-Cyanoquinoline

CAS Registry Number: 67360-38-7

Molecular Formula: C₁₀H₆N₂

Molecular Weight: 154.171

Accurate Mass: 154.053098

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

Physical Description: Pale brown cryst.

Melting Point: Mp 104°

References:

Hirsch, J.A. *et al.*, *J.O.C.*, 1974, **39**, 2044, (*synth*)