



>>Entry Name: 8-Quinolinecarboxylic acid, 9CI

CAS Registry Number: 86-59-9

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: Used as 1% soln. in dil. NaOH for extraction-photometric detn. of Fe(II) (in the presence of Py, CHCl₃, pH 3-6)

Physical Description: Needles (H₂O)

Melting Point: Mp 187°

pKa Value: pK_{a1} 2.01; pK_{a2} 6.84 (25°, 0.1M NaClO₄)

Aldrich: 36779-6

>>Derivative: Me ester

CAS Registry Number: 40245-26-9

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%

Boiling Point: Bp_{0.5} 129-131°

>>Derivative: Et ester

CAS Registry Number: 25635-22-7

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 45°

Boiling Point: Bp₁₃ 194-197°. Bp_{0.3} 145-155°

>>Derivative: Amide

CAS Registry Number: 55706-61-1

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. (H₂O)

Melting Point: Mp 171-173°

>>Derivative: Nitrile

Synonym(s): 8-Quinolinecarbonitrile, 9CI. 8-Cyanoquinoline

CAS Registry Number: 35509-27-4

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 84°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **3**, 448A, (*nmr*)
Elderfield, R.C. *et al.*, *J.A.C.S.*, 1951, **73**, 5622, (*synth*)
Lumme, P.O., *Suom. Kemistil. B*, 1957, **30**, 204, (*ir*)
Zehner, J.M. *et al.*, *Anal. Chim. Acta*, 1966, **35**, 135, (*detn, Fe*)
Kovi, P.J. *et al.*, *Anal. Chim. Acta*, 1972, **62**, 59, (*uv*)
Anderson, B.A. *et al.*, *J.O.C.*, 1998, **63**, 8224-8228, (*nitrile, synth, ir, pmr, cmr*)