



>>Entry Name: 4,7-Dichloroquinoline, 9Cl

CAS Registry Number: 86-98-6

Molecular Formula: C₉H₅Cl₂N

Molecular Weight: 198.051

Accurate Mass: 196.979903

Percentage Composition: C 54.58%; H 2.54%; Cl 35.80%; N 7.07%

Physical Description: Needles (EtOH) or cryst. (MeOH)

Melting Point: Mp 86.4-87.4°. Mp 93°

Boiling Point: Bp₅ 125°

pKa Value: pK_a 2.8 (25°)

Aldrich: 14143-7

Fluka: 35610

Sigma: D6274

>>Derivative: Methiodide

CAS Registry Number: 39844-54-7

Physical Description: Yellow powder

Melting Point: Mp 240-242°

>>Derivative: Tribromide

CAS Registry Number: 12365-92-3

Molecular Formula: C₉H₆Br₃Cl₂N

Molecular Weight: 438.771

Accurate Mass: 434.802736

Percentage Composition: C 24.64%; H 1.38%; Br 54.63%; Cl 16.16%; N 3.19%

Physical Description: Cryst.

Melting Point: Mp 140-142°

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 857D, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 429A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1569B, (*ir*)
Andersag, H., *Chem. Ber.*, 1948, **81**, 499-507, (*synth*)
Kwart, H. *et al.*, *J.A.C.S.*, 1958, **80**, 884-887, (*synth*)
Fr. Pat., 1968, 1 514 280; *CA*, **70**, 68195t, (*synth*)
Simonyi, I., *Magy. Kem. Foly.*, 1968, **74**, 311, (*tribromide*)
Ger. Pat., 1982, 3 112 415; *CA*, **98**, 71952w, (*synth*)
Galanakis, D. *et al.*, *J. Med. Chem.*, 1996, **39**, 359-370, (*methiodide, synth, pmr*)