



>>Entry Name: 5-Isoquinolinol, 9Cl

Synonym(s): 5-Hydroxyisoquinoline

CAS Registry Number: 2439-04-5

Molecular Formula: C₉H₇NO

Molecular Weight: 145.16

Accurate Mass: 145.052764

Percentage Composition: C 74.47%; H 4.86%; N 9.65%; O 11.02%

Physical Description: Cryst.

Melting Point: Mp 225-228°

pKa Value: pK_{a1} 5.38; pK_{a2} 8.47 (20°)

Aldrich: H3320-7

>>Derivative: N-Me betaine

>>Derivative: Benzyl ether

CAS Registry Number: 61672-52-4

Molecular Formula: C₁₆H₁₃NO

Molecular Weight: 235.285

Accurate Mass: 235.099714

Percentage Composition: C 81.68%; H 5.57%; N 5.95%; O 6.80%

Physical Description: Purple solid

Melting Point: Mp 58-62°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 878D, (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 753B, (*nmr*)

Koelsch, C.F. *et al.*, *J.A.C.S.*, 1953, **75**, 2095, (*synth*)