



>>Entry Name: 5-Quinolinol
Synonym(s): 5-Hydroxyquinoline

CAS Registry Number: 578-67-6
Related CAS Registry Numbers(s): 1321-40-0

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: Plates
Melting Point: Mp 224°
pKa Value: pK_{a1} 5.18; pK_{a2} 8.56 (20°)

Aldrich: 12879-1
Fluka: 55065

>>Derivative: Me ether
Synonym(s): 5-Methoxyquinoline

CAS Registry Number: 6931-19-7
Molecular Formula: C₁₀H₉NO
Molecular Weight: 159.187
Accurate Mass: 159.068414
Percentage Composition: C 75.45%; H 5.70%; N 8.80%; O 10.05%
Boiling Point: Bp₁₂ 181-185°

>>Derivative: Me ether, N-oxide

Molecular Formula: C₁₀H₉NO₂
Molecular Weight: 175.187
Accurate Mass: 175.063329
Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%
Melting Point: Mp 106-107°

>>Derivative: Et ether
Synonym(s): 5-Ethoxyquinoline

Molecular Formula: C₁₁H₁₁NO
Molecular Weight: 173.214
Accurate Mass: 173.084064
Percentage Composition: C 76.28%; H 6.40%; N 8.09%; O 9.24%
Boiling Point: Bp₁₅ 160°

>>Derivative: N-Oxide

Molecular Formula: C₉H₇NO₂
Molecular Weight: 161.16
Accurate Mass: 161.047679
Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%
Physical Description: Yellow cryst. (MeOH)
Melting Point: Mp 215° (dec.)

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 859C, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 432A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1570B, (*ir*)
Bradford, L. *et al.*, *J.C.S.*, 1947, 437, (*synth, deriv*)
Palmer, M.H., *J.C.S.*, 1962, 3645, (*synth, deriv*)
Tamura, Y. *et al.*, *Chem. Ind. (London)*, 1970, 1435, (*synth*)
Yokoyama, A. *et al.*, *Chem. Pharm. Bull.*, 1997, **45**, 279, (*N-oxide*)