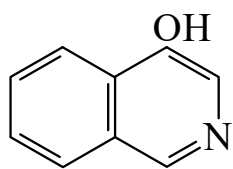




>>Entry Name: 4-Isoquinolinol, 9CI

Synonym(s): 4-Hydroxyisoquinoline



CAS Registry Number: 3336-49-0

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: Cryst.

Melting Point: Mp 223-224 dec.°

pKa Value: pK_{a1} 4.78; pK_{a2} 8.7 (20°)

>>Derivative: Hydrochloride

CAS Registry Number: 15365-53-4

Physical Description: Cryst.

Melting Point: Mp 139-140°

>>Derivative: Methiodide

Physical Description: Cryst.

Melting Point: Mp 151°

>>Derivative: 4-Methylbenzenesulfonyl

Physical Description: Cryst. (MeOH)

Melting Point: Mp 92-93°

>>Derivative: Me ether

Synonym(s): 4-Methoxyisoquinoline

CAS Registry Number: 36034-54-5

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%

Physical Description: Prisms (Et₂O)

Melting Point: Mp 72-73°

>>Derivative: Me ether, N-oxide

CAS Registry Number: 76570-11-1

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%

Physical Description: Needles (C₆H₆)

Melting Point: Mp 184-185°

References:

Ochiai, E. *et al.*, *Chem. Pharm. Bull.*, 1955, **3**, 454-458, (*synth*)

Kimoto, S. *et al.*, *Chem. Pharm. Bull.*, 1972, **20**, 10-14, (*Me ether, synth*)

Albini, A. *et al.*, *J.C.S. Perkin 1*, 1980, 2738-2742, (*Me ether N-oxide, synth, pmr*)