



>>Entry Name: 3-Methylisoquinoline, 9CI

CAS Registry Number: 1125-80-0

Molecular Formula: C₁₀H₉N

Molecular Weight: 143.188

Accurate Mass: 143.073499

Percentage Composition: C 83.88%; H 6.34%; N 9.78%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 68°

Boiling Point: Bp 246°. Bp_{0.2} 60°

pKa Value: pK_a 5.64 (25°)

Hazard & Toxicity: Fl. p. 106°

Aldrich: 12989-5

Rare Chemicals Library: S44296-8

>>Derivative: Picrate

Physical Description: Yellow needles

Melting Point: Mp 197-198°

Solubility: Spar. sol. H₂O

>>Derivative: Methiodide

Physical Description: Golden needles (EtOH)

Melting Point: Mp 219°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 457A, (*nmr*)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1401C, (*ir*)

Mills, W.H. *et al.*, *J.C.S.*, 1922, **121**, 2732

Tirodkar, R.B. *et al.*, *Indian J. Chem.*, 1972, **10**, 1060

Ribar, B. *et al.*, *Cryst. Struct. Commun.*, 1974, **3**, 323, (*cryst struct*)

Su, J.A. *et al.*, *Org. Magn. Reson.*, 1977, **10**, 122, (*cmr*)

Pitts, M.R. *et al.*, *J.C.S. Perkin 1*, 2001, 955-977, (*methiodide, pmr*)