



>>Entry Name: 5-Fluoro-1*H*-indole, 9CI

CAS Registry Number: 399-52-0

Structure by analogy with 3-Fluoro-1*H*-indole, [HFN19-E](#)

Molecular Formula: C₈H₆FN

Molecular Weight: 135.14

Accurate Mass: 135.048427

Percentage Composition: C 71.10%; H 4.47%; F 14.06%; N 10.36%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 46-47°

pKa Value: pK_a 16.3

Aldrich: F910-8

Fluka: 47080

Sigma: F1751

>>Derivative: Picrate

Physical Description: Orange cryst. (C₆H₆)

Melting Point: Mp 155-156°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 125C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1500C, (*ir*)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1244C, (*ir*)

Allen, F.L. *et al.*, *J.C.S.*, 1955, 1283, (*synth, uv, derivs*)

Pelchowicz, Z. *et al.*, *J.C.S.*, 1961, 5418, (*synth*)

Hoffmann, E. *et al.*, *J. Het. Chem.*, 1965, **2**, 298, (*synth*)

Yagil, G., *Tetrahedron*, 1967, **23**, 2855, (*props*)

Lallemand, J.Y. *et al.*, *Bull. Soc. Chim. Fr.*, 1970, **11**, 4091, (*pmr*)

Sirowe, H. *et al.*, *Synthesis*, 1972, 84, (*synth*)

Rosenberg, E. *et al.*, *Org. Magn. Reson.*, 1976, **8**, 117, (*N-15 nmr, cmr*)

Ayachit, N.H. *et al.*, *Spectrochim. Acta A*, 1986, **42**, 781, (*ir, uv*)