



>>Entry Name: 5-Nitroindole

CAS Registry Number: 6146-52-7

Molecular Formula: $C_8H_6N_2O_2$

Molecular Weight: 162.148

Accurate Mass: 162.042928

Percentage Composition: C 59.26%; H 3.73%; N 17.28%; O 19.73%

Physical Description: Yellow solid or needles (C_6H_6 /cyclohexane)

Melting Point: Mp 140-141° (134-137°)

pKa Value: pK_{a1} -7.4; pK_{a2} 14.75 (25°,NH, KOH aq.)

Aldrich: N1760-2

Fluka: 73415

Sigma: N7751

>>Derivative: 1-Me

Synonym(s): 1-Methyl-5-nitro-1*H*-indole

CAS Registry Number: 29906-67-0

Molecular Formula: $C_9H_8N_2O_2$

Molecular Weight: 176.174

Accurate Mass: 176.058578

Percentage Composition: C 61.36%; H 4.58%; N 15.90%; O 18.16%

Physical Description: Yellow solid

Melting Point: Mp 164°

pKa Value: pK_a -6.6

Other Data: Subl. at 112°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 665B, (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 524C, (*nmr*)

Thesing, J. *et al.*, *Chem. Ber.*, 1962, **95**, 2205, (*synth, uv*)

Challis, B.C. *et al.*, *J.C.S. Perkin 2*, 1973, 918, (*props, deriv*)

Russell, H.F. *et al.*, *Org. Prep. Proced. Int.*, 1985, **17**, 391, (*synth*)

Vance, W.A. *et al.*, *Mutat. Res.*, 1986, **173**, 169, (*deriv*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, NHK500