



>>Entry Name: 4-Nitroindole

CAS Registry Number: 4769-97-5

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%

Use/Importance: Intermed. in natural prod. synthesis

Physical Description: Yellow prisms (MeOH aq.)

Melting Point: Mp 206-207°

Aldrich: 26996-4

>>Derivative: 1-Me

CAS Registry Number: 91482-63-2

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%

Melting Point: Mp 112-116°

>>Derivative: 1-Et

Molecular Formula: $C_{10}H_{10}N_2O_2$

Molecular Weight: 190.201

Accurate Mass: 190.074228

Percentage Composition: C 63.15%; H 5.30%; N 14.73%; O 16.82%

Melting Point: Mp 50.5°

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 665A, (*ir*)
Parmerter, S.M. *et al.*, *J.A.C.S.*, 1958, **80**, 4621, (*synth*, *uv*)
Somei, M. *et al.*, *Chem. Pharm. Bull.*, 1981, **29**, 726, (*synth*, *ir*, *pmr*)
Org. Synth., 1987, **65**, 146, (*synth*)
Girgis, N.J. *et al.*, *J. Het. Chem.*, 1988, **25**, 361, (*synth*)
Melhado, L.L. *et al.*, *J.O.C.*, 1988, **53**, 3852, (*synth*, *pmr*)
Bergman, J. *et al.*, *Tetrahedron*, 1990, **46**, 6085; 6113, (*deriv*)