



>>Entry Name: 5-Nitroisoquinoline

CAS Registry Number: 607-32-9

Molecular Formula: $C_9H_6N_2O_2$

Molecular Weight: 174.159

Accurate Mass: 174.042928

Percentage Composition: C 62.07%; H 3.47%; N 16.08%; O 18.37%

Physical Description: Long yellow needles (EtOH)

Melting Point: Mp 110°

Aldrich: 13022-2

>>Derivative: 2-Oxide

CAS Registry Number: 57554-78-6

Molecular Formula: $C_9H_6N_2O_3$

Molecular Weight: 190.158

Accurate Mass: 190.037843

Percentage Composition: C 56.85%; H 3.18%; N 14.73%; O 25.24%

Physical Description: Yellow needles (Me₂CO)

Melting Point: Mp 220-222°

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **3**, 459B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 866D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1573B, (*ir*)

Ochiai, E. *et al.*, *Yakugaku Zasshi*, 1953, **73**, 666; *CA*, **48**, 7014b

Dewar, M.J.S. *et al.*, *J.C.S.*, 1957, 2521, (*synth*)

Henry, R.A. *et al.*, *J.O.C.*, 1972, **37**, 3206, (*synth*, *pmr*)

Potts, K.T. *et al.*, *J.O.C.*, 1986, **51**, 2011, (*synth*)