



>>Entry Name: 4-Nitroquinoline

CAS Registry Number: 3741-15-9

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%

Melting Point: Mp 87°

Hazard & Toxicity: Mutagen. Noncarcinogenic

>>Derivative: N-Oxide

CAS Registry Number: 56-57-5

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: Yellowish-brown plates or needles

Melting Point: Mp 154°

Hazard & Toxicity: Exp. carcinogen. Potent mutagen

Aldrich: 21844-8

Fluka: 73265

Rare Chemicals Library: S57291-8

Sigma: N8141

Supelco: 44-2683

References:

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 779D, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 919A, (ir)

Filippi, J., *Bull. Soc. Chim. Fr.*, 1968, 259, (synth, ir, uv)

Carcinog. - Compr. Surv., (ed., Sugimura, T.), Vol. 6 The Nitroquinolines, Raven Press, New York, 1981, (book)

Woodgate, P.D. *et al.*, *Heterocycles*, 1987, **26**, 1029, (synth)

Demeunynck, M. *et al.*, *J.O.C.*, 1989, **54**, 399; 405, (tox, bibl)

Yokoyama, A. *et al.*, *Chem. Pharm. Bull.*, 1997, **45**, 279-283, (N-oxide)

Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., Van Nostrand Reinhold, 1979, 866

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, NJF000