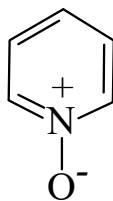




>>Entry Name: Pyridine N-oxide



CAS Registry Number: 694-59-7

Molecular Formula: C₅H₅NO

Molecular Weight: 95.101

Accurate Mass: 95.037114

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

Use/Importance: Reagent for oxidative decarboxylation of α -halo acids and carboxylic acids to aldehydes. Used as 20% aq. soln. (acidified with HCl) for extraction-photometric detn. of Au

Physical Description: Solid

Melting Point: Mp 65-66°

Boiling Point: Bp 270°. Bp₁₅ 136-140°. Bp₁ 100-105°

pKa Value: pK_a 0.82 (2428°, H₂O 24) pK_a 0.79 (25°, H₂SO₄ aq.)

Hazard & Toxicity: LD₅₀ (mus, ipr) 1425 mg/kg

Aldrich: 13165-2

Fluka: 82811

>>Derivative: Hydrochloride

CAS Registry Number: 16527-88-1

Physical Description: Cryst. (2-propanol)

Melting Point: Mp 179.5-181°

>>Derivative: Picrate

Physical Description: Yellow needles

Melting Point: Mp 180.5-182°

>>Derivative: Methyl perchlorate

CAS Registry Number: 4329-79-7

Physical Description: Cryst. (EtOH)

Melting Point: Mp 69-70°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 912C, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1575B, (ir)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 773A, (nmr)

Org. Synth., 1953, **33**, 79, (synth)

Eisenthal, R. *et al.*, *Tetrahedron*, 1965, **21**, 2205, (reactions)

Holt, P.F. *et al.*, *J.C.S.(B)*, 1968, 233, (uv)

Ziegler, M. *et al.*, *Mikrochim. Acta*, 1970, 628, (detn, Au)

Ulku, D. *et al.*, *Acta Cryst. B*, 1971, **27**, 432, (cryst struct)

Tamura, Y. *et al.*, *Chem. Pharm. Bull.*, 1971, **19**, 130, (synth)

Tolstikov, G.A. *et al.*, *Tet. Lett.*, 1971, 2807, (synth)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 567

Cowan, D.A. *et al.*, *Biomed. Mass Spectrom.*, 1978, **5**, 551, (ms)

Wamsler, T. *et al.*, *J. Magn. Reson.*, 1978, **31**, 177, (pmr, cmr)

Kireev, G.V. *et al.*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1980, 1034, (ir, uv)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, POS000

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 1733