



>>Entry Name: 3-Methylpyridine, 9CI

Synonym(s): 3-Picoline, 8CI. β -Picoline

CAS Registry Number: 108-99-6

Extra CAS Registry Numbers(s): 1333-41-1

Molecular Formula: C_6H_7N

Molecular Weight: 93.128

Accurate Mass: 93.057849

Percentage Composition: C 77.38%; H 7.58%; N 15.04%

Physical Description: Oil with sweetish odour

Boiling Point: Bp 143.8°

Solubility: Misc. most solvs.

Density: d_4^{25} 0.952

pKa Value: pK_a 5.7 (25°)

Refractive Index: n_D^{25} 1.5043

Hazard & Toxicity: Flammable, fl. p. 40°. Irritant. Adverse CNS effects by inhalation. LD₅₀ (rat, ipr) 150 mg/kg

Aldrich: P4205-3

Fluka: 80230

>>Derivative: Methiodide

CAS Registry Number: 10129-51-8

Melting Point: Mp 92°

Rare Chemicals Library: S61939-6

>>Derivative: Picrate

Melting Point: Mp 149-150°

>>Derivative: N-Oxide

CAS Registry Number: 1003-73-2

Molecular Formula: C_6H_7NO

Molecular Weight: 109.127

Accurate Mass: 109.052764

Percentage Composition: C 66.04%; H 6.47%; N 12.84%; O 14.66%

Melting Point: Mp 33-35°

Boiling Point: Bp₁₅ 150°

pKa Value: pK_a 1.08

Aldrich: P4240-1

Fluka: 80270

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **3**, 244B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 735B; 913A, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1516D; 1575D, (ir)

Henze, M., *Ber.*, 1934, **67**, 750, (synth)

Riethof, G. *et al.*, *Ind. Eng. Chem., Anal. Ed.*, 1946, **18**, 458, (purifn)

Cullinane, N.M. *et al.*, *J. Soc. Chem. Ind., London*, 1948, **67**, 142, (synth)

Coulson, E.A. *et al.*, *J.C.S.*, 1954, 1957, (synth)

Weissberger, A., *Chem. Heterocycl. Compd.*, 1960, **14**, 99

Cole, W.G. *et al.*, *J.C.S.(B)*, 1968, 1284, (ms)

Cushley, R.J. *et al.*, *Can. J. Chem.*, 1975, **53**, 3419, (cmr)

Marker, A. *et al.*, *Aust. J. Chem.*, 1978, **31**, 1255, (pmr)

Denisov, A.Y. *et al.*, *Khim. Geterotsikl. Soedin.*, 1984, **20**, 1223, (cmr, pmr)

Handa, T. *et al.*, *J. Phys. Chem.*, 1986, **90**, 2589, (uv)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, PIB920

Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 225

Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, 1992, 868