



>>Entry Name: 4-Acetylpyridine

Synonym(s): 1-(4-Pyridinyl)ethanone, 9Cl. Methyl 4-pyridyl ketone. 4-Acetopyridine

CAS Registry Number: 1122-54-9

Molecular Formula: C₇H₇NO

Molecular Weight: 121.138

Accurate Mass: 121.052764

Percentage Composition: C 69.41%; H 5.82%; N 11.56%; O 13.21%

Use/Importance: Acetylcholine antagonist. Organoleptic.

Physical Description: Liq.

Boiling Point: Bp 212-214°

pKa Value: pK_a 3.51 (25°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 1400 mg/kg

Aldrich: A2140-1

Fluka: 1450

Sigma: A7524

>>Derivative: Picrate

Physical Description: Leaflets

Melting Point: Mp 129-130°

>>Derivative: Oxime

CAS Registry Number: 1194-99-6

Molecular Formula: C₇H₈N₂O

Molecular Weight: 136.153

Accurate Mass: 136.063663

Percentage Composition: C 61.75%; H 5.92%; N 20.57%; O 11.75%

Melting Point: Mp 142°

Rare Chemicals Library: S10147-8

>>Derivative: Phenylhydrazone

CAS Registry Number: 39585-84-7

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 150°

>>Derivative: Semicarbazone

Melting Point: Mp 218-219°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 313A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 781D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1543B, (*ir*)

Marvel, C.S. *et al.*, *J.O.C.*, 1955, **20**, 1785, (*synth*)

Isaac, R. *et al.*, *Appl. Spectrosc.*, 1963, **17**, 90, (*uv*)

Retcofsky, M.L. *et al.*, *J. Phys. Chem.*, 1967, **71**, 3592, (*cmr*)

Katritzky, A.R. *et al.*, *J.A.C.S.*, 1969, **91**, 636, (*ir*)

Lessman, T. *et al.*, *Org. Mass Spectrom.*, 1973, **7**, 1321, (*ms*)

Kasende, O. *et al.*, *J. Het. Chem.*, 1985, **22**, 1647, (*ir, props*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, ADA 365