



>>Entry Name: 3-Acetylpyridine

ENTRY UNDER REVIEW

Synonym(s): 1-(3-Pyridinyl)ethanone, 9Cl. Methyl 3-pyridyl ketone. 3-Acetopyridine. FEMA 3424

CAS Registry Number: 350-03-8

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: Organoleptic in cigarette smoke

Physical Description: Liq.

Boiling Point: Bp 220°. Bp₁₂ 106°

Solubility: Sol. H₂O

pKa Value: pK_a 3.26 (25°)

Other Data: Yellows in air.

Aldrich: W34240-8

Fluka: 1440

Sigma: A5001

>>Derivative: Hydrochloride

Melting Point: Mp 80 dec.°

>>Derivative: Oxime

CAS Registry Number: 5973-83-1

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 130.5°

>>Derivative: Phenylhydrazone

Melting Point: Mp 137°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 312B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 780C, (*ir*)

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

Scott, F.L., *J.O.C.*, 1957, **22**, 1568, (*synth*)

Katritzky, A.R. *et al.*, *J.C.S.*, 1958, 3165, (*uv*)

Kavalewski, V.J., *J. Chem. Phys.*, 1962, **36**, 266, (*pmr*)

Miyajama, G. *et al.*, *Chem. Pharm. Bull.*, 1972, **20**, 429, (*cmr*)

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

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, ABI000