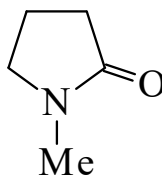




>>Entry Name: 1-Methyl-2-pyrrolidinone, 9CI

Synonym(s): N-Methylpyrrolidone



CAS Registry Number: 872-50-4

Extra CAS Registry Numbers(s): 51013-18-4

Molecular Formula: C₅H₉NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Biological Source: Alkaloid from *Melicope hayesii*

Use/Importance: Dipolar aprotic solvent, with low oral acute tox. Weakly basic, good proton acceptor from strong acids

Melting Point: Mp -17° (-24°)

Boiling Point: Bp 202°. Bp₁₀ 85°

Solubility: Sol. H₂O, most org. solvs.

Density: d₄²⁰ 1.027

pKa Value: pK_a -0.92 (H₂SO₄ aq.)

Refractive Index: n_D²⁵ 1.4690

Other Data: Steam-volatile. Forms hydrates

Hazard & Toxicity: Fl. p. 96° (oc), autoignition temp. 346°. Severe eye irritant. Exp. reprod. and teratogenic effects. OES: long-term 100 ppm

Aldrich: 27045-8

Fluka: 69120

Sigma: M6762

>>Derivative: Hydrochloride

CAS Registry Number: 16889-93-3

Melting Point: Mp 79-81°

>>Derivative: Oxime

CAS Registry Number: 35197-40-1

Molecular Formula: C₅H₁₀N₂O

Molecular Weight: 114.147

Accurate Mass: 114.079313

Percentage Composition: C 52.61%; H 8.83%; N 24.54%; O 14.02%

Melting Point: Mp 98-99°

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 789C, (ir)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1286A, (nmr)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 788D, (ir)
Fery, L.P.A. *et al.*, *Bull. Soc. Chim. Belg.*, 1960, **69**, 63, (synth)
Blicke, F.F. *et al.*, *J.O.C.*, 1961, **26**, 1826, (synth)
Metzger, H. *et al.*, *Angew. Chem., Int. Ed.*, 1963, **2**, 624, (synth)
Falbe, J. *et al.*, *Chem. Ber.*, 1965, **98**, 1928, (synth)
Basch, H. *et al.*, *J. Chem. Phys.*, 1968, **49**, 5007, (uv)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 281
Fronza, G. *et al.*, *J.C.S. Perkin 2*, 1977, 1746, (N-15 nmr, cmr)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **19**, 514
Cerioni, G. *et al.*, *Spectrochim. Acta A*, 1983, **39**, 929, (pmr, cmr)
Ruostesuo, P. *et al.*, *Spectrochim. Acta A*, 1985, **41**, 739, (cmr, N-15 nmr, O-17 nmr)
Ermakov, A.I. *et al.*, *Zh. Org. Khim.*, 1985, **21**, 1986, (ms)
Tyman, J. *et al.*, *Synth. Commun.*, 1989, **19**, 179, (use)
Latip, J. *et al.*, *Phytochemistry*, 1999, **51**, 107-110, (isol, pmr, cmr)
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. *et al.*), J.B. Lippincott, 1988, 344
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, 1992, 869
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MPF200