



>>Entry Name: 3-Acetylpyrrole

Synonym(s): 1-(1*H*-Pyrrol-3-yl)ethanone, 9CI. Methyl 3-pyrrol ketone. 3-Acetopyrrole

CAS Registry Number: 1072-82-8

Molecular Formula: C₆H₇NO

Molecular Weight: 109.127

Accurate Mass: 109.052764

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

Physical Description: Cryst. (CHCl₃/petrol)

Melting Point: Mp 115-116°

>>Derivative: *N*-Me

CAS Registry Number: 932-62-7

Molecular Formula: C₇H₉NO

Molecular Weight: 123.154

Accurate Mass: 123.068414

Percentage Composition: C 68.27%; H 7.37%; N 11.37%; O 12.99%

Boiling Point: Bp₁₅ 148-150°

Refractive Index: n_D²⁰ 1.5380

Aldrich: 30986-9

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 6A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1447D, (*ir*)

Khan, M.K.A. *et al.*, *Tetrahedron*, 1966, **22**, 2095, (*synth*)

Loader, C.E. *et al.*, *Tetrahedron*, 1969, **25**, 3879, (*synth, pmr*)

v. Leusen, A.M. *et al.*, *Tet. Lett.*, 1972, 5337, (*synth*)

Anderson, H.J. *et al.*, *Synth. Commun.*, 1987, **17**, 401, (*synth*)

Pindur, U. *et al.*, *J. Het. Chem.*, 1989, **26**, 1563, (*ir*)