



>>Entry Name: 3,5-Dimethylisoxazole, 9CI

CAS Registry Number: 300-87-8

Structure by analogy with 3,4-Dimethylisoxazole, [GBW59-W](#)

Molecular Formula: C₅H₇NO

Molecular Weight: 97.116

Accurate Mass: 97.052764

Percentage Composition: C 61.84%; H 7.26%; N 14.42%; O 16.47%

Boiling Point: Bp₇₄₈ 141-142°. Bp₂₉ 49-50°

pKa Value: pK_a -1.26

Aldrich: D16750-9

Sigma: D2266

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 97B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 635B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1488D, (*ir*)

Lampe, W., *Pol. J. Chem. (Rocz. Chem.)*, 1954, **28**, 163, (*synth*)

Fitton, A.O. *et al.*, *Practical Heterocyclic Chemistry*, Academic Press, N.Y., 1968, 28

Kashima, C. *et al.*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 310, (*synth*)

Yavari, I. *et al.*, *J.O.C.*, 1975, **40**, 2880, (*synth, nmr*)