



>>Entry Name: 4-Methylpyridazine, 9CI

CAS Registry Number: 1120-88-3

Molecular Formula: $C_5H_6N_2$

Molecular Weight: 94.116

Accurate Mass: 94.053098

Percentage Composition: C 63.81%; H 6.43%; N 29.76%

Boiling Point: Bp₂₇ 119°

Density: d²⁰ 1.064

pKa Value: pK_a 3.53 (17°)

Refractive Index: n_D²⁰ 1.5145

Aldrich: 29777-1

>>Derivative: 1-Oxide

CAS Registry Number: 21004-76-2

Molecular Formula: $C_5H_6N_2O$

Molecular Weight: 110.115

Accurate Mass: 110.048013

Percentage Composition: C 54.54%; H 5.49%; N 25.44%; O 14.53%

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 83-84°

>>Derivative: 2-Oxide

CAS Registry Number: 21004-77-3

Molecular Formula: $C_5H_6N_2O$

Molecular Weight: 110.115

Accurate Mass: 110.048013

Percentage Composition: C 54.54%; H 5.49%; N 25.44%; O 14.53%

Physical Description: Hygroscopic solid

Boiling Point: Bp₄ 135°

>>Derivative: 1,2-Dioxide

Molecular Formula: $C_5H_6N_2O_2$

Molecular Weight: 126.115

Accurate Mass: 126.042928

Percentage Composition: C 47.62%; H 4.80%; N 22.21%; O 25.37%

Physical Description: Cryst. (Me₂O/EtOH)

Melting Point: Mp 150-150.5°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 355A, (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1550C, (ir)

Schmidt, P. *et al.*, *Helv. Chim. Acta*, 1954, **37**, 1467, (synth)

Mizzoni, R.H. *et al.*, *J.A.C.S.*, 1954, **76**, 2201, (synth)

Tori, K. *et al.*, *Chem. Pharm. Bull.*, 1964, **12**, 272, (nmr)

Ogura, H. *et al.*, *J. Het. Chem.*, 1971, **8**, 391, (ms)