>>**Entry Name: 4-Nitropyridine**

CAS Registry Number: 1122-61-8

Molecular Formula: $C_5H_4N_2O_2$
Molecular Weight: 124.099
Accurate Mass: 124.027278
Percentage Composition: C 48.39%; H 3.25%; N 22.57%; O 25.78%
Physical Description: Plates (EtOH aq.)
Melting Point: Mp 50°
pKa Value: pK_a 1.61 (20°)

>>**Derivative:** *N*-Oxide

CAS Registry Number: 1124-33-0
Molecular Formula: $C_5H_4N_2O_3$
Molecular Weight: 140.098
Accurate Mass: 140.022193
Percentage Composition: C 42.87%; H 2.88%; N 20.00%; O 34.26%
Physical Description: Pale-yellow rhombic cryst. (EtOH)
Melting Point: Mp 159-160°
Aldrich: 34665-9
Sigma: N1393

>>**Derivative:** 1-Me

CAS Registry Number: 200799-00-4
Molecular Formula: $C_6H_7N_2O_2^{(+)}$
Molecular Weight: 139.134
Accurate Mass: 139.050753
Percentage Composition: C 51.80%; H 5.07%; N 20.13%; O 23.00%
Physical Description: Pale yellow needles (as tetrafluoroborate)
Melting Point: Mp 130° (tetrafluoroborate)
Other Data: CAS no. refers to tetrafluoroborate

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 916A, *(ir)*
Kroehnke, F. *et al.*, *Chem. Ber.*, 1962, **95**, 1098
Wang, Y. *et al.*, *Acta Cryst. B*, 1976, **32**, 572, *(cryst struct, oxide)*
Negele, S. *et al.*, *J.O.C.*, 1998, **63**, 1138-1143, *(1-Me, synth, pmr)*
Lewis, R.J.*, Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NJA500