



>>Entry Name: 4-Pyridinecarboxaldehyde, 9Cl
Synonym(s): Isonicotinaldehyde, 8Cl. 4-Formylpyridine

CAS Registry Number: 872-85-5
Related CAS Registry Numbers(s): 696-53-7 1637-52-1

Molecular Formula: C₆H₅NO
Molecular Weight: 107.112
Accurate Mass: 107.037114
Percentage Composition: C 67.28%; H 4.70%; N 13.08%; O 14.94%
Physical Description: Oil
Boiling Point: Bp₁₆ 82-83°
Solubility: Sol. H₂O
Density: d₄²⁰ 1.137
pKa Value: pK_{a1} 4.77; pK_{a2} 12.2 (20°, 0.2M KNO₃)
Refractive Index: n_D²⁵ 1.5352

Aldrich: P6240-2
Fluka: 82730
Sigma: P8130

>>Derivative: Picrate

Physical Description: Cryst. + 1H₂O
Melting Point: Mp 168-169°

>>Derivative: Methiodide

CAS Registry Number: 13441-53-7
Melting Point: Mp 114-116°

>>Derivative: Oxime
Synonym(s): 4-Pyridinealdoxime

CAS Registry Number: 696-54-8
Molecular Formula: C₆H₆N₂O
Molecular Weight: 122.126
Accurate Mass: 122.048013
Percentage Composition: C 59.01%; H 4.95%; N 22.94%; O 13.10%
Physical Description: Cryst. (H₂O)
Melting Point: Mp 131°
pKa Value: pK_{a2} 9.6 (25°, NOH, 0.5M KNO₃)

Aldrich: 13162-8
Fluka: 82780
Sigma: P8630

>>Derivative: Phenylhydrazone

CAS Registry Number: 7757-39-3

Molecular Formula: C₁₂H₁₁N₃
Molecular Weight: 197.239
Accurate Mass: 197.095297
Percentage Composition: C 73.07%; H 5.62%; N 21.30%
Use/Importance: Used as a 0.1% soln. in EtOH as acid-base indicator
Physical Description: Cryst. (MeOH aq.)
Melting Point: Mp 178-179°. Mp 157°
pKa Value: pK_{a1} 5.89 (20% EtOH)
Rare Chemicals Library: S32097-8

>>Derivative: Phenylhydrazone; hydrochloride

Melting Point: Mp 270°