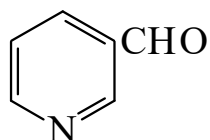




>>Entry Name: 3-Pyridinecarboxaldehyde, 9CI  
Synonym(s): Nicotinaldehyde, 8CI. 3-Formylpyridine



CAS Registry Number: 500-22-1

Molecular Formula: C<sub>6</sub>H<sub>5</sub>NO  
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: Bp<sub>26</sub> 97-99°. Bp<sub>11</sub> 83-87°  
Solubility: Sol. H<sub>2</sub>O, EtOH, Me<sub>2</sub>CO, CHCl<sub>3</sub>; insol. Et<sub>2</sub>O  
Density: d<sub>4</sub><sup>20</sup> 1.415  
pKa Value: pK<sub>a1</sub> 3.8; pK<sub>a2</sub> 13.1 (20°, 0.2M KNO<sub>3</sub>)  
Refractive Index: n<sub>D</sub><sup>20</sup> 1.5498  
Hazard & Toxicity: Appears to be a strong skin irritant

Aldrich: P6220-8  
Fluka: 82720  
Sigma: P8005

>>Derivative: Methochloride

Melting Point: Mp 105°

>>Derivative: Methiodide

CAS Registry Number: 13441-54-8  
Physical Description: Yellow cryst.  
Melting Point: Mp 174°

>>Derivative: Oxime  
Synonym(s): 3-Pyridinealdoxime

CAS Registry Number: 1193-92-6  
Molecular Formula: C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O  
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.  
Melting Point: Mp 150°  
pKa Value: pK<sub>a2</sub> 10.17 (25°)  
Hazard & Toxicity: LD<sub>50</sub> (mus, ipr) 200 mg/kg

Aldrich: P5840-5

>>Derivative: Hydrazone

Molecular Formula: C<sub>6</sub>H<sub>7</sub>N<sub>3</sub>  
Molecular Weight: 121.141  
Accurate Mass: 121.063997  
Percentage Composition: C 59.49%; H 5.82%; N 34.69%  
Use/Importance: Used as 0.01M aq. soln. for photometric detn. of V(I) (λ<sub>max</sub> 420 nm, ε 750)  
Physical Description: Hygroscopic cryst.  
Melting Point: Mp 35°  
Solubility: Sol. EtOH, C<sub>6</sub>H<sub>6</sub>; spar. sol. H<sub>2</sub>O

>>Derivative: Phenylhydrazone

CAS Registry Number: 57023-37-7  
Physical Description: Cryst. (EtOH)  
Melting Point: Mp 158°