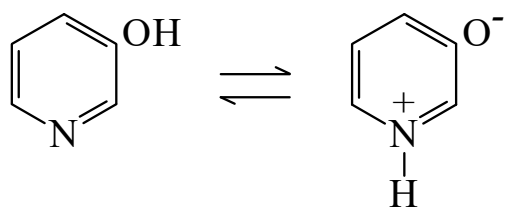




>>Entry Name: 3-Pyridinol

Synonym(s): 3-Hydroxypyridine. 3-Pyridol



CAS Registry Number: 109-00-2

Molecular Formula: C₅H₅NO

Molecular Weight: 95.101

Accurate Mass: 95.037114

Percentage Composition: C 63.15%; H 5.30%; N 14.73%; O 16.82%

Use/Importance: Reagent used in peptide synth.

Physical Description: Needles

Melting Point: Mp 129°

pKa Value: pK_{a1} 4.79; pK_{a2} 8.75 (20°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 1822 mg/kg

Aldrich: H5700-9

Fluka: 56390

Sigma: H2512

>>Derivative: Tartaric ester

Synonym(s): Hydroxypyridine tartrate, INN

CAS Registry Number: 7008-17-5

Molecular Formula: C₉H₉NO₆

Molecular Weight: 227.173

Accurate Mass: 227.042989

Percentage Composition: C 47.58%; H 3.99%; N 6.17%; O 42.26%

Use/Importance: Peripheral vasodilator

Development Status: Never marketed

Melting Point: Mp 155.5-157° (as picrate)

Calculated Log P Data: Log P -2.51 (calc)

>>Derivative: O-Ac

Synonym(s): 3-Acetoxypyridine

CAS Registry Number: 17747-43-2

Molecular Formula: C₇H₇NO₂

Molecular Weight: 137.138

Accurate Mass: 137.047679

Percentage Composition: C 61.31%; H 5.14%; N 10.21%; O 23.33%

Use/Importance: Mild acetylating agent for alcohols, phenols and amines

Melting Point: Mp 155.5-157° (as picrate)

Boiling Point: Bp₅₈ 137°

>>Derivative: N-Me, zwitterion

Synonym(s): 3-Hydroxy-1-methylpyridinium hydroxide inner salt, 9CI

CAS Registry Number: 25065-00-3

Molecular Formula: C₆H₇NO

Molecular Weight: 109.127

Accurate Mass: 109.052764

Percentage Composition: C 66.04%; H 6.47%; N 12.84%; O 14.66%

Physical Description: Hygroscopic needles (EtOH)

Melting Point: Mp 37-38°