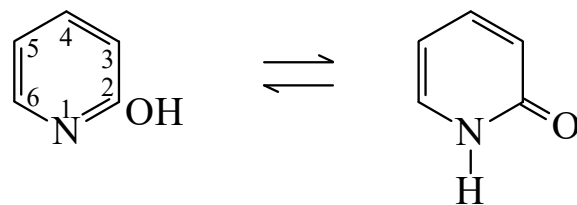




>>Entry Name: **2(1*H*)-Pyridinone**, 9CI

Synonym(s): 2(1*H*)-Pyridone, 8CI. α -Pyridone. 2-Hydroxypyridine. 2-Pyridinol. α -Pyridol. 2-Pyridol



CAS Registry Number: 142-08-5

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: Catalyses condensations. Used in peptide synth.

Physical Description: Needles (C₆H₆)

Melting Point: Mp 106-107°

Boiling Point: Bp 280-281°

pKa Value: pK_{a1} 0.75; pK_{a2} 11.65 (20°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 410 mg/kg

Aldrich: H5680-0

Fluka: 56380

Sigma: H7758

>>Derivative: *N*-Oxide

Synonym(s): 1-Hydroxy-2(1*H*)-pyridinone

CAS Registry Number: 822-89-9

Extra CAS Registry Numbers(s): 13161-30-3

Molecular Formula: C₅H₅NO₂

Molecular Weight: 111.1

Accurate Mass: 111.032029

Percentage Composition: C 54.05%; H 4.54%; N 12.61%; O 28.80%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 148-150°

Other Data: *N*-Hydroxypyridone struct. predominates in cryst. struct. and soln.

>>Variant: *NH*-form

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%

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-2(1*H*)-pyridinone

CAS Registry Number: 694-85-9

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: Oil

Boiling Point: Bp₁₀ 117°

Refractive Index: n_D²⁰ 1.5685

Aldrich: M7825-9

Fluka: 69072

>>Derivative: *N*-Me, picrate

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 145° (142-143°)