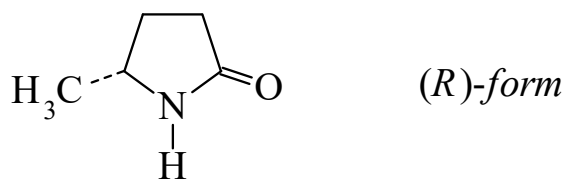




>>Entry Name: 5-Methyl-2-pyrrolidinone, 9Cl, 8Cl

Synonym(s): γ -Valerolactam



CAS Registry Number: 108-27-0

Related CAS Registry Numbers(s): 1558-60-7

Molecular Formula: C₅H₉NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Aldrich: M7970-0

>>Variant: (R)-form

CAS Registry Number: 21395-93-7

Molecular Formula: C₅H₉NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Physical Description: Oil

Boiling Point: Bp₃ 66°

Optical Rotation: $[\alpha]_D^{20} +26.6$ (H₂O)

>>Derivative: 1-Chloromethyl

CAS Registry Number: 154747-82-7

Molecular Formula: C₆H₁₀ClNO

Molecular Weight: 147.604

Accurate Mass: 147.045091

Percentage Composition: C 48.82%; H 6.83%; Cl 24.02%; N 9.49%; O 10.84%

Use/Importance: Reagent for determination of enantiomeric compn. of alcohols

Physical Description: Liq.

Boiling Point: Bp₆ 99°

Optical Rotation: $[\alpha]_D^{20} +109.9$ (c, 0.032 in CHCl₃) (>99% ee)

>>Variant: (S)-form

CAS Registry Number: 1558-60-7

Molecular Formula: C₅H₉NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Optical Rotation: $[\alpha]_D^{20} -26.6$ (c, 0.9 in H₂O)

>>Variant: (±)-form

CAS Registry Number: 62182-32-5

Molecular Formula: C₅H₉NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Physical Description: Hygroscopic cryst.

Melting Point: Mp 41-43°

Boiling Point: Bp₇ 119-120°

>>Derivative: Hydrochloride

CAS Registry Number: 62069-49-2

Physical Description: Needles (Et₂O)

Melting Point: Mp 110°

>>Derivative: N-Ac