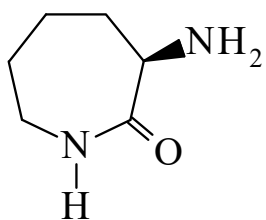




>>Entry Name: 3-Aminohexahydro-2*H*-azepin-2-one, 9Cl

Synonym(s): 3-Amino-ε-caprolactam



(*R*)-form

CAS Registry Number: 671-42-1

Molecular Formula: C₆H₁₂N₂O

Molecular Weight: 128.174

Accurate Mass: 128.094963

Percentage Composition: C 56.23%; H 9.44%; N 21.86%; O 12.48%

>>Variant: (*R*)-form

CAS Registry Number: 28957-33-7

Molecular Formula: C₆H₁₂N₂O

Molecular Weight: 128.174

Accurate Mass: 128.094963

Percentage Composition: C 56.23%; H 9.44%; N 21.86%; O 12.48%

Sigma: A5537

>>Derivative: Hydrochloride

CAS Registry Number: 26081-03-8

Physical Description: Solid (MeOH)

Optical Rotation: $[\alpha]_{\text{D}}^{26} +26.4$ (c, 4 in 1*M* HCl) (>99% ee)

>>Derivative: Hydrobromide

CAS Registry Number: 16473-63-5

Optical Rotation: $[\alpha]_{\text{D}}^{20} +20.7$ (c, 5 in H₂O)

>>Variant: (*S*)-form

CAS Registry Number: 21568-87-6

Molecular Formula: C₆H₁₂N₂O

Molecular Weight: 128.174

Accurate Mass: 128.094963

Percentage Composition: C 56.23%; H 9.44%; N 21.86%; O 12.48%

Melting Point: Mp 71-72°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -34$ (c, 4 in 1*M* HCl) (100% ee)

Aldrich: 26359-1

Fluka: 7257

Sigma: A5412

>>Derivative: Hydrochloride

CAS Registry Number: 26081-07-2

Melting Point: Mp 270°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -27$ (c, 2.98 in 1*M* HCl)

>>Derivative: Hydrobromide

CAS Registry Number: 16473-62-4

Melting Point: Mp 285-288 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -20.7$ (c, 5 in H₂O)