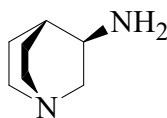




>>Entry Name: 1-Azabicyclo[2.2.2]octan-3-amine, 9Cl

Synonym(s): 3-Amino-1-azabicyclo[2.2.2]octane. 3-Aminoquinuclidine



(R)-form

CAS Registry Number: 6238-14-8

Molecular Formula: C₇H₁₄N₂

Molecular Weight: 126.201

Accurate Mass: 126.115698

Percentage Composition: C 66.62%; H 11.18%; N 22.20%

>>Variant: (R)-form

CAS Registry Number: 123536-15-2

Molecular Formula: C₇H₁₄N₂

Molecular Weight: 126.201

Accurate Mass: 126.115698

Percentage Composition: C 66.62%; H 11.18%; N 22.20%

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 123536-14-1

Physical Description: Cryst. (HCl aq./EtOH)

Optical Rotation: $[\alpha]_D^{20} +24.8$ (c, 1 in H₂O)

Other Data: Mp >285°

Aldrich: 41571-5

Sigma: A1202

>>Derivative: 3-N-Ac

CAS Registry Number: 134869-61-7

Molecular Formula: C₉H₁₆N₂O

Molecular Weight: 168.238

Accurate Mass: 168.126263

Percentage Composition: C 64.25%; H 9.59%; N 16.65%; O 9.51%

Melting Point: Mp 128-130°

Optical Rotation: $[\alpha]_D^{20} +49.5$ (c, 2 in CHCl₃) (99.3% op)

>>Variant: (S)-form

CAS Registry Number: 120570-05-0

Molecular Formula: C₇H₁₄N₂

Molecular Weight: 126.201

Accurate Mass: 126.115698

Percentage Composition: C 66.62%; H 11.18%; N 22.20%

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 119904-90-4

Physical Description: Cryst.

Optical Rotation: $[\alpha]_D^{20} -24.9$ (c, 1 in H₂O)

Other Data: Mp >285°

Aldrich: 41572-3

Sigma: A1327

>>Derivative: 3-N-Ac

CAS Registry Number: 134869-59-3

Melting Point: Mp 128-131°

Optical Rotation: $[\alpha]_D^{20} -50$ (c, 2 in CHCl₃) (99.5% op)