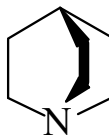




>>Entry Name: 1-Azabicyclo[2.2.2]octane, 9CI

Synonym(s): Quinuclidine, 8CI. Nuclidine



CAS Registry Number: 100-76-5

Molecular Formula: C₇H₁₃N

Molecular Weight: 111.186

Accurate Mass: 111.104799

Percentage Composition: C 75.62%; H 11.78%; N 12.60%

Use/Importance: Base used in org. synth. Forms cryst. complexes with organolithium compds.

Physical Description: Cryst. with ammoniacal odour

Melting Point: Mp 158° (sealed tube)

Solubility: V. sol. H₂O

pKa Value: pK_a 6.74 (22°)

Other Data: Very volatile

Aldrich: 19760-2

Fluka: 22709

>>Derivative: Hydrochloride

CAS Registry Number: 39896-06-5

Physical Description: Cryst. (EtOH)

Melting Point: Mp 364-365°

Aldrich: 13591-7

Fluka: 22712

>>Derivative: Hydrobromide

CAS Registry Number: 60662-68-2

Physical Description: Cryst.

Melting Point: Mp 325-330 dec.°

>>Derivative: Picrate

Physical Description: Pale-yellow needles (EtOH)

Melting Point: Mp 275 dec.°

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-1-azoniabicyclo[2.2.2]octane(1+)

CAS Registry Number: 3618-94-8

Molecular Formula: C₈H₁₆N⁽⁺⁾

Molecular Weight: 126.221

Accurate Mass: 126.128274

Percentage Composition: C 76.13%; H 12.78%; N 11.10%

Physical Description: Cryst. (Et₂O/EtOH) (as iodide)

Melting Point: Mp 357-358° (iodide)

Other Data: CAS no. refers to iodide

>>Derivative: *N*-Et

Synonym(s): 1-Ethyl-1-azoniabicyclo[2.2.2]octane(1+)

CAS Registry Number: 3618-93-7

Molecular Formula: C₉H₁₈N⁽⁺⁾

Molecular Weight: 140.248

Accurate Mass: 140.143924

Percentage Composition: C 77.08%; H 12.94%; N 9.99%

Physical Description: Plates (EtOH) (as iodide)

Melting Point: Mp 270-271° (iodide)

Other Data: Slightly hygroscopic. CAS no. refers to iodide

References: