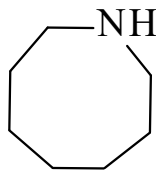




>>Entry Name: Octahydroazocine, 9CI

Synonym(s): Perhydroazocine. Azacyclooctane. Heptamethyleneimine



CAS Registry Number: 1121-92-2

Molecular Formula: C₇H₁₅N

Molecular Weight: 113.202

Accurate Mass: 113.120449

Percentage Composition: C 74.27%; H 13.36%; N 12.37%

Boiling Point: Bp₃₀ 75-77°

Density: d₄²¹ 0.896

pKa Value: pK_a 9.77

Refractive Index: n_D²¹ 1.4740

Aldrich: H215-5

Fluka: 51710

>>Derivative: Hydrochloride

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 177°

>>Derivative: 4-Methylbenzenesulfonyl

Melting Point: Mp 82.5°

>>Derivative: 1-Me

CAS Registry Number: 19719-81-4

Molecular Formula: C₈H₁₇N

Molecular Weight: 127.229

Accurate Mass: 127.136099

Percentage Composition: C 75.52%; H 13.47%; N 11.01%

Melting Point: Mp 215° (as picrate)

>>Derivative: 1-Et

CAS Registry Number: 73676-23-0

Molecular Formula: C₉H₁₉N

Molecular Weight: 141.256

Accurate Mass: 141.151749

Percentage Composition: C 76.53%; H 13.56%; N 9.92%

Melting Point: Mp 163° (as picrate)

>>Derivative: 1-Isopropyl

CAS Registry Number: 108696-11-3

Molecular Formula: C₁₀H₂₁N

Molecular Weight: 155.283

Accurate Mass: 155.167399

Percentage Composition: C 77.35%; H 13.63%; N 9.02%

Melting Point: Mp 141° (as picrate)

>>Derivative: 1-*tert*-Butyl

CAS Registry Number: 108696-12-4

Molecular Formula: C₁₁H₂₃N

Molecular Weight: 169.309

Accurate Mass: 169.183049

Percentage Composition: C 78.04%; H 13.69%; N 8.27%

Melting Point: Mp 159° (as picrate)

References: