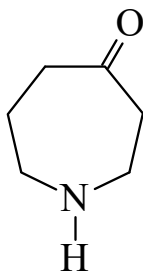




>>Entry Name: Hexahydro-4*H*-azepin-4-one, 9CI

Synonym(s): Perhydroazepin-4-one



CAS Registry Number: 105416-56-6

Related CAS Registry Numbers(s): 50492-22-3

Molecular Formula: C₆H₁₁NO

Molecular Weight: 113.159

Accurate Mass: 113.084064

Percentage Composition: C 63.69%; H 9.80%; N 12.38%; O 14.14%

>>Derivative: Hydrochloride

CAS Registry Number: 19869-42-2

Physical Description: Solid (EtOH)

Melting Point: Mp 166.5-167° (160° dec.)

Boiling Point: Bp₃ 97-100° (lit. gives a pressure range)

>>Derivative: Picrate

Physical Description: Solid

Melting Point: Mp 151-152°

>>Derivative: *N*-Me

CAS Registry Number: 1859-33-2

Molecular Formula: C₇H₁₃NO

Molecular Weight: 127.186

Accurate Mass: 127.099714

Percentage Composition: C 66.11%; H 10.30%; N 11.01%; O 12.58%

Physical Description: Liq.

Boiling Point: Bp₄₅ 115-120°

Density: d₂₃ 0.963

Refractive Index: n_D²³ 1.4893

Other Data: Rapidly darkens on standing

>>Derivative: *N*-Me, picrate

Physical Description: Cryst. (Me₂CO/MeOH)

Melting Point: Mp 171-172°

References:

Diamirol, J. *et al.*, *J.O.C.*, 1965, **30**, 1840, (*synth, deriv*)

Polivka, Z. *et al.*, *Coll. Czech. Chem. Comm.*, 1986, **51**, 2034, (*synth*)

Laronze, J.Y. *et al.*, *Synth. Commun.*, 1991, **21**, 881, (*synth, derivs*)

Roglans, A. *et al.*, *Synth. Commun.*, 1992, **22**, 1429, (*synth*)