



CAS Registry Number: 114636-31-6
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%
Physical Description: Oil

>>Derivative: 3-*N*-Me

CAS Registry Number: 144043-19-6
Molecular Formula: C₅H₁₂N₂
Molecular Weight: 100.163
Accurate Mass: 100.100048
Percentage Composition: C 59.96%; H 12.08%; N 27.97%
Optical Rotation: [α]_D +3.4 (c, 0.5 in 0.1*N* HCl) (as hydrochloride)
Other Data: CAS no. refers to hydrochloride

>>Derivative: 3-*N,N*-Di-Me

CAS Registry Number: 144043-20-9
Extra CAS Registry Numbers(s): 132883-44-4
Molecular Formula: C₆H₁₄N₂
Molecular Weight: 114.19
Accurate Mass: 114.115698
Percentage Composition: C 63.11%; H 12.36%; N 24.53%
Optical Rotation: [α]_D -2.8 (c, 0.5 in MeOH aq.) (hydrochloride)
Other Data: CAS no. refers to hydrochloride

>>Derivative: 1-Benzyl

CAS Registry Number: 114715-38-7
Molecular Formula: C₁₁H₁₆N₂
Molecular Weight: 176.261
Percentage Composition: C 74.96%; H 9.15%; N 15.89%
Physical Description: Oil

>>Derivative: 1-Benzyl, 3-*N*-Ac

CAS Registry Number: 114636-30-5
Molecular Formula: C₁₃H₁₈N₂O
Molecular Weight: 218.298
Accurate Mass: 218.141913
Percentage Composition: C 71.53%; H 8.31%; N 12.83%; O 7.33%
Physical Description: Red oil
Optical Rotation: [α]_D²⁰ -19 (c, 1.0 in CHCl₃)

>>Variant: (±)-form

Molecular Formula: C₄H₁₀N₂
Molecular Weight: 86.136
Accurate Mass: 86.084398
Percentage Composition: C 55.78%; H 11.70%; N 32.52%

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 103831-11-4
Melting Point: Mp 300°
Aldrich: 40462-4
Sigma: A2567

References:

Rosen, T. *et al.*, *J. Med. Chem.*, 1988, **31**, 1586, (*synth*, *pmr*)
Di Cesare, P. *et al.*, *J. Med. Chem.*, 1992, **35**, 4205, (*synth*, *pmr*)