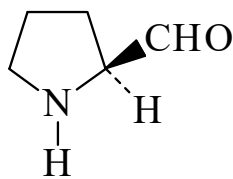




>>Entry Name: 2-Pyrrolidinecarboxaldehyde

Synonym(s): 2-Formylpyrrolidine. Prolinal



CAS Registry Number: 61480-98-6

Molecular Formula: C₅H₉NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

>>Variant: (S)-form

CAS Registry Number: 88218-12-6

Molecular Formula: C₅H₉NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

>>Derivative: Diethyl dithioacetal

CAS Registry Number: 105089-88-1

Molecular Formula: C₉H₁₉NS₂

Molecular Weight: 205.388

Accurate Mass: 205.095889

Percentage Composition: C 52.63%; H 9.32%; N 6.82%; S 31.22%

Physical Description: Pale-yellow oil

Optical Rotation: $[\alpha]_D^{23} -31.8$ (c, 0.434 in CHCl₃)

>>Derivative: N-Benzyloxycarbonyl

CAS Registry Number: 71461-30-8

Molecular Formula: C₁₃H₁₅NO₃

Molecular Weight: 233.266

Accurate Mass: 233.105194

Percentage Composition: C 66.94%; H 6.48%; N 6.00%; O 20.58%

Optical Rotation: $[\alpha]_D^{24} -74.42$ (c, 0.138 in CHCl₃)

>>Derivative: *tert*-Butyloxycarbonyl

CAS Registry Number: 69610-41-9

Extra CAS Registry Numbers(s): 59378-82-4 73365-02-3 117625-90-8

Molecular Formula: C₁₀H₁₇NO₃

Molecular Weight: 199.249

Accurate Mass: 199.120844

Percentage Composition: C 60.28%; H 8.60%; N 7.03%; O 24.09%

Use/Importance: Important intermediate in peptide synth.

Physical Description: Pale yellow liq.

Other Data: (*R*)-enantiomer also known

References:

- Evans, D.A. *et al.*, *J.A.C.S.*, 1979, **101**, 371-378, (*S-tert-butyloxycarbonyl*)
Becker, Y. *et al.*, *J.O.C.*, 1980, **45**, 2145-2151, (*R-tert-butyloxycarbonyl*)
Frick, L. *et al.*, *Biochim. Biophys. Acta*, 1985, **529**, 311, (*synth, biochem*)
Langley, D.R. *et al.*, *J.O.C.*, 1987, **52**, 91, (*deriv, synth, pmr, ir, ms*)
McNulty, J. *et al.*, *Synth. Commun.*, 1992, **22**, 979-985, (*S-tert-butyloxycarbonyl*)
Drew, M.G.B. *et al.*, *J.C.S. Perkin 1*, 1998, 1627-1636, (*N-benzyl, N-Boc*)