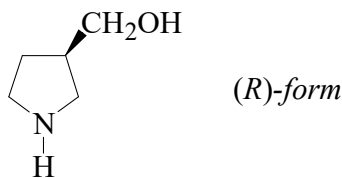




>>Entry Name: 3-Pyrrolidinemethanol, 9CI

Synonym(s): 3-(Hydroxymethyl)pyrrolidine. β -Prolinol



CAS Registry Number: 5082-74-6

Molecular Formula: $C_5H_{11}NO$

Molecular Weight: 101.148

Accurate Mass: 101.084064

Percentage Composition: C 59.37%; H 10.96%; N 13.85%; O 15.82%

>>Variant: (R)-form

CAS Registry Number: 110013-18-8

Molecular Formula: $C_5H_{11}NO$

Molecular Weight: 101.148

Accurate Mass: 101.084064

Percentage Composition: C 59.37%; H 10.96%; N 13.85%; O 15.82%

Melting Point: Mp 92-95°

Optical Rotation: $[\alpha]_D^{25} +26.6$ (c, 6.0 in EtOH)

Other Data: Also descr. as an oil

>>Variant: (S)-form

CAS Registry Number: 110013-19-9

Molecular Formula: $C_5H_{11}NO$

Molecular Weight: 101.148

Accurate Mass: 101.084064

Percentage Composition: C 59.37%; H 10.96%; N 13.85%; O 15.82%

Physical Description: Oil

Boiling Point: Bp_{0.08} 100°

Optical Rotation: $[\alpha]_D^{25} -26$ (c, 6.0 in EtOH)

>>Derivative: N-Benzyl

CAS Registry Number: 78914-69-9

Molecular Formula: $C_{12}H_{17}NO$

Molecular Weight: 191.272

Accurate Mass: 191.131014

Percentage Composition: C 75.35%; H 8.96%; N 7.32%; O 8.36%

Physical Description: Oil

Boiling Point: Bp_{0.08} 110°

Optical Rotation: $[\alpha]_D^{25} -3.1$ (c, 4.1 in EtOH)

References:

Fleš, D. *et al.*, *Croat. Chem. Acta*, 1964, **36**, 27-32, (*synth*)

Culbertson, T.P. *et al.*, *J. Med. Chem.*, 1987, **30**, 1711-1715, (*R-form*, *S-form*, *synth*)

Mazzini, C. *et al.*, *J.O.C.*, 1997, **62**, 5215-5218, (*R-form*, *S-form*, *synth*, *pmr*, *cmr*, *ir*, *ms*)