



>>Entry Name: *N*-Alanylvaline

CAS Registry Number: 1472-66-8

Extra CAS Registry Numbers(s): 1999-46-8

H3CCH(NH2)CONHCH(COOH)CH(CH3)2

Molecular Formula: C₈H₁₆N₂O₃

Molecular Weight: 188.226

Accurate Mass: 188.116093

Percentage Composition: C 51.05%; H 8.57%; N 14.88%; O 25.50%

Rare Chemicals Library: S78906-2

>>Variant: D-D-form

Molecular Formula: C₈H₁₆N₂O₃

Molecular Weight: 188.226

Accurate Mass: 188.116093

Percentage Composition: C 51.05%; H 8.57%; N 14.88%; O 25.50%

>>Derivative: *N*-Benzyloxycarbonyl

Melting Point: Mp 149-150°

Optical Rotation: $[\alpha]_{\text{D}}^{23} +23$ (c, 2.0 in MeOH) (lit. gives a temp. range)

>>Variant: L-L-form

CAS Registry Number: 3303-45-5

Molecular Formula: C₈H₁₆N₂O₃

Molecular Weight: 188.226

Accurate Mass: 188.116093

Percentage Composition: C 51.05%; H 8.57%; N 14.88%; O 25.50%

Sigma: A4253

>>Derivative: *N*-Benzyloxycarbonyl

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 122-125°

Optical Rotation: $[\alpha]_{\text{D}}^{22} -12.8$ (c, 3.6 in EtOH)

>>Variant: L-D-form

Molecular Formula: C₈H₁₆N₂O₃

Molecular Weight: 188.226

Accurate Mass: 188.116093

Percentage Composition: C 51.05%; H 8.57%; N 14.88%; O 25.50%

Physical Description: Needles or prisms (EtOH)

Melting Point: Mp 265°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -5.9$ (H₂O). $[\alpha]_{\text{D}}^{20} -1.9$ (HCl)

References:

Fischer, E. *et al.*, *Annalen*, 1908, **363**, 148, (*synth*)

Weygand, F. *et al.*, *Chem. Ber.*, 1960, **93**, 2983

Parker, F.S., *Prog. Infrared Spectrosc.*, 1967, **3**, 89, (*ir*)

Nicolaides, E. *et al.*, *J. Med. Chem.*, 1968, **11**, 74