



Physical Description: Plates (H₂O) or rhombs (Me₂CO)
Melting Point: Mp 164-165°
Optical Rotation: $[\alpha]_D^{25} -3.4$ (EtOH). $[\alpha]_D^{25} -9.36$ (AcOH). $[\alpha]_D^{25} +20.05$ (H₂O)
Sigma: A6876

>>Derivative: *N*-Benzoyl, Me ester

CAS Registry Number: 1492-13-3
Molecular Formula: C₁₃H₁₇NO₃
Molecular Weight: 235.282
Accurate Mass: 235.120844
Percentage Composition: C 66.36%; H 7.28%; N 5.95%; O 20.40%
Melting Point: Mp 109-109.5°
Optical Rotation: $[\alpha]_D^{23} -43$ (CHCl₃)

>>Derivative: *N*-4-Methylbenzenesulfonyl

Melting Point: Mp 149.5-150.5°
Optical Rotation: $[\alpha]_D^{22} -27.7$ (EtOH)

>>Derivative: *N*-(4-Hydroxycinnamoyl)
Synonym(s): *N-p*-Coumaroyl-D-valine

CAS Registry Number: 155179-33-2

Molecular Formula: C₁₄H₁₇NO₄
Molecular Weight: 263.293
Accurate Mass: 263.115759
Percentage Composition: C 63.87%; H 6.51%; N 5.32%; O 24.31%
Biological Source: Isol. from yeast-elicited *Ephedra distachya*

>>Derivative: *N*-Me
Synonym(s): *N*-Methylvaline, 9Cl, 8Cl

Molecular Formula: C₆H₁₃NO₂
Molecular Weight: 131.174
Accurate Mass: 131.094629
Percentage Composition: C 54.94%; H 9.99%; N 10.68%; O 24.39%
Melting Point: Mp 171-173° (as hydrochloride)
Optical Rotation: $[\alpha]_D^{20} -26.5$ (hydrochloride)

>>Variant: (*S*)-form
Synonym(s): L-form

CAS Registry Number: 72-18-4

Molecular Formula: C₅H₁₁NO₂
Molecular Weight: 117.147
Accurate Mass: 117.078979
Percentage Composition: C 51.26%; H 9.46%; N 11.96%; O 27.31%
Biological Source: Widely distributed in nature as one of the principal protein amino acids
Use/Importance: Dietary supplement
Physical Description: Plates (EtOH aq.)
Melting Point: Mp 315 dec.° (sealed tube)
Optical Rotation: $[\alpha]_D^{20} +6.3$ (H₂O). $[\alpha]_D^{20} +23.4$ (1*M* HCl). $[\alpha]_D^{20} +27.6$ (6*M* HCl)
Solubility: Sol. H₂O (8.85 g per 100 cm³ at 25°); spar. sol. EtOH
pKa Value: p*K*_{a1} 2.32; p*K*_{a2} 9.62 (NH₂)
Other Data: Isoelectric point 5.96. Bitter taste

Aldrich: V70-5
Fluka: 94619
Sigma: V5628

>>Derivative: Hydrochloride

CAS Registry Number: 17498-50-9
Optical Rotation: $[\alpha]_D^{20} +27.54$