



>>Entry Name: Alanylalanine

Extra CAS Registry Numbers(s): 2867-20-1 59247-16-4
H3CCH(NH2)CONHCH(CH3)COOH

Molecular Formula: C₆H₁₂N₂O₃
Molecular Weight: 160.172
Accurate Mass: 160.084793
Percentage Composition: C 44.99%; H 7.55%; N 17.49%; O 29.97%

>>Variant: D-D-form

CAS Registry Number: 923-16-0
Molecular Formula: C₆H₁₂N₂O₃
Molecular Weight: 160.172
Accurate Mass: 160.084793
Percentage Composition: C 44.99%; H 7.55%; N 17.49%; O 29.97%
Optical Rotation: [α]_D²⁵+21.3 (c, 2 in H₂O). [α]_D²⁴+37.9 (c, 2 in 0.5*M* HCl)
Sigma: A0912

>>Variant: D-L-form

CAS Registry Number: 1115-78-2
Molecular Formula: C₆H₁₂N₂O₃
Molecular Weight: 160.172
Accurate Mass: 160.084793
Percentage Composition: C 44.99%; H 7.55%; N 17.49%; O 29.97%
Melting Point: Mp 269-270 dec.°
Optical Rotation: [α]_D²⁰−68.5

>>Variant: L-D-form

CAS Registry Number: 3695-80-5
Molecular Formula: C₆H₁₂N₂O₃
Molecular Weight: 160.172
Accurate Mass: 160.084793
Percentage Composition: C 44.99%; H 7.55%; N 17.49%; O 29.97%
Melting Point: Mp 275-276°
Optical Rotation: [α]_D²⁵+67.2 (c, 2 in 6*M* HCl)

>>Variant: L-L-form

CAS Registry Number: 1948-31-8
Molecular Formula: C₆H₁₂N₂O₃
Molecular Weight: 160.172
Accurate Mass: 160.084793
Percentage Composition: C 44.99%; H 7.55%; N 17.49%; O 29.97%
Physical Description: Prisms
Melting Point: Mp 298°
Optical Rotation: [α]_D²⁵−38.3 (c, 2 in 6*M* HCl)
Aldrich: 85679-7
Fluka: 5250
Sigma: A9502

>>Derivative: Me ester

Molecular Formula: C₇H₁₄N₂O₃
Molecular Weight: 174.199
Accurate Mass: 174.100443
Percentage Composition: C 48.26%; H 8.10%; N 16.08%; O 27.55%
Melting Point: Mp 126-128°
Optical Rotation: [α]_D²⁵−35.9 (c, 1.0 in EtOH)