



CAS Registry Number: 19436-52-3
Molecular Formula: C₅H₉NO₃
Molecular Weight: 131.131
Accurate Mass: 131.058244
Percentage Composition: C 45.80%; H 6.92%; N 10.68%; O 36.60%
Melting Point: Mp 125°
Optical Rotation: [α]_D +66.5 (c, 2 in H₂O)
Sigma: A4375

>>Derivative: *N*-Benzoyl

CAS Registry Number: 17966-60-8
Molecular Formula: C₁₀H₁₁NO₃
Molecular Weight: 193.202
Accurate Mass: 193.073894
Percentage Composition: C 62.17%; H 5.74%; N 7.25%; O 24.84%
Melting Point: Mp 151°
Optical Rotation: [α]_D -37.3 (c, 0.8 in KOH)
Rare Chemicals Library: S45506-7
Sigma: B0504

>>Derivative: *N*-*tert*-Butyloxycarbonyl

CAS Registry Number: 7764-95-6
Molecular Formula: C₈H₁₅NO₄
Molecular Weight: 189.211
Accurate Mass: 189.100109
Percentage Composition: C 50.78%; H 7.99%; N 7.40%; O 33.82%
Physical Description: Cryst. (EtOAc/pentane)
Melting Point: Mp 80-81°
Optical Rotation: [α]_D²⁰ +24.6 (c, 2 in AcOH)

>>Derivative: *N*-Me

Synonym(s): *N*-Methylalanine, 9CI. 2-(Methylamino)propanoic acid

CAS Registry Number: 29475-64-7
Molecular Formula: C₄H₉NO₂
Molecular Weight: 103.121
Accurate Mass: 103.063329
Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%
Physical Description: Needles + 1H₂O (EtOH)
Melting Point: Mp *ca.* 300°
Optical Rotation: [α]_D²⁰ -5.9 (H₂O)
Sigma: M7524

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 56-41-7

Molecular Formula: C₃H₇NO₂
Molecular Weight: 89.094
Accurate Mass: 89.047679
Percentage Composition: C 40.44%; H 7.92%; N 15.72%; O 35.92%
Biological Source: Obt. from hydrolysates of many proteins. Most proteins contain about 9% alanine
Use/Importance: A non-essential aminoacid
Biological Use/Importance: Dietary supplement, nutrient
Melting Point: Mp 297 dec.°
Optical Rotation: [α]_D +14.6 (c, 1 in 5*M* HCl). [α]_D +1.8 (c, 1 in H₂O)
Solubility: Insol. EtOH; sol. H₂O (16.5g/100ml at 25°)
pKa Value: p*K*_{a1} 2.34; p*K*_{a2} 9.69 (NH₂)
Other Data: Isoelectric point 6.01. Sweet taste

Aldrich: A2680-2

Fluka: 5130

Sigma: A5824