



Accurate Mass: 165.078979
Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%
Biological Source: Widely distributed in proteins
Biological Use/Importance: Dietary supplement, nutrient
Physical Description: Needles (H₂O)
Melting Point: Mp 283-284° (rapid heat)
Optical Rotation: $[\alpha]_D^{20} -34.3$ (c, 1 in H₂O) (98% op)
Solubility: Spar. sol. H₂O (2.97 g/100 g at 25°)
pKa Value: pK_{a2} 9.13 (NH₂)
Other Data: Isoelectric point 5.48. Bitter taste
Hazard & Toxicity: LD₅₀ (rat, ipr) 5287 mg/kg

Aldrich: W35850-9

Fluka: 78019

Sigma: P3923

>>Derivative: Me ester; hydrochloride

CAS Registry Number: 7524-50-7
Extra CAS Registry Numbers(s): 2577-90-4
Melting Point: Mp 159-161°
Optical Rotation: $[\alpha]_D^{25} -4.6$ (c, 5 in H₂O)
Aldrich: P1720-2
Fluka: 78090
Sigma: P3126

>>Derivative: Et ester; hydrochloride

CAS Registry Number: 3182-93-2
Extra CAS Registry Numbers(s): 3081-24-1
Physical Description: Cryst. (EtOH/Et₂O)
Melting Point: Mp 159-161°
Optical Rotation: $[\alpha]_D^{25} -4.6$ (c, 5 in H₂O). $[\alpha]_D^{21} +36.8$ (c, 4.8 in EtOH)
Aldrich: 22070-1
Fluka: 78050
Sigma: P2751

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 16874-17-2
Molecular Formula: C₁₃H₁₉NO₂
Molecular Weight: 221.299
Accurate Mass: 221.141579
Percentage Composition: C 70.56%; H 8.65%; N 6.33%; O 14.46%
Physical Description: Liq.
Boiling Point: Bp_{0.25} 107°
Optical Rotation: $[\alpha]_D^{25} +24.6$ (neat)
Density: d₄²⁰ 1.02
Refractive Index: n_D²⁰ 1.4970

>>Derivative: *tert*-Butyl ester, hydrochloride

CAS Registry Number: 15100-75-1
Physical Description: Cryst.
Melting Point: Mp 207-208 dec.°
Optical Rotation: $[\alpha]_D^{25} +45.2$ (c, 2 in EtOH)

>>Derivative: Benzyl ester

CAS Registry Number: 962-39-0
Molecular Formula: C₁₆H₁₇NO₂
Molecular Weight: 255.316
Accurate Mass: 255.125929
Percentage Composition: C 75.27%; H 6.71%; N 5.49%; O 12.53%