



Fluka: 5703
Sigma: I8754

>>Derivative: Me ester

CAS Registry Number: 42271-58-9
Molecular Formula: C₇H₁₅NO₂
Molecular Weight: 145.201
Percentage Composition: C 57.90%; H 10.41%; N 9.65%; O 22.04%
Physical Description: Oil

>>Derivative: Et ester

CAS Registry Number: 44975-82-8
Molecular Formula: C₈H₁₇NO₂
Molecular Weight: 159.228
Accurate Mass: 159.125929
Percentage Composition: C 60.35%; H 10.76%; N 8.80%; O 20.10%
Melting Point: Mp 89-90° (as hydrochloride)
Optical Rotation: [α]_D²⁵+15 (c, 1 in H₂O)

>>Derivative: Amide; hydrochloride

CAS Registry Number: 63328-67-6
Melting Point: Mp 240-241 dec.°
Optical Rotation: [α]_D²⁵+32 (c, 1 in H₂O)

>>Derivative: *N*-Formyl

Melting Point: Mp 126° (123°)
Optical Rotation: [α]_D²⁰+24.2 (EtOH). [α]_D²⁶+27.9 (c, 2 in EtOH)

>>Derivative: *N*-Ac

CAS Registry Number: 20257-17-4
Melting Point: Mp 155-156°
Optical Rotation: [α]_D²⁵-5.3 (c, 2 in H₂O). [α]_D+21.5 (c, 2 in EtOH)

>>Derivative: *N*-Benzenesulfonyl

Melting Point: Mp 147-148°
Optical Rotation: [α]_D²⁰+30.7 (EtOH)

>>Variant: (2*S*,3*S*)-form
Synonym(s): L-*erythro*-form. L-Isoleucine

CAS Registry Number: 73-32-5

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%
Biological Source: Found in hydrolysates of proteins and peptides
Use/Importance: Dietary supplement, nutrient
Physical Description: Cryst. (EtOH aq.)
Melting Point: Mp 285-286 dec.°
Optical Rotation: [α]_D+16.3 (H₂O). [α]_D+51.8 (5*M* HCl)
Solubility: Mod. sol. H₂O (4.12 g/100 g at 25°)
pKa Value: p*K*_{a1} 2.36; p*K*_{a2} 9.68 (NH₂)
Other Data: Isoelectric point 6.02. Bitter taste

Aldrich: 15171-8
Fluka: 58880
Sigma: I2752