



Fluka: 5703
Sigma: I8754

>>Derivative: Me ester

CAS Registry Number: 42271-58-9
Molecular Formula: $C_7H_{15}NO_2$
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: $C_8H_{17}NO_2$
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: $[\alpha]_D^{25} +15$ (c, 1 in H_2O)

>>Derivative: Amide; hydrochloride

CAS Registry Number: 63328-67-6
Melting Point: Mp 240-241 dec.°
Optical Rotation: $[\alpha]_D^{25} +32$ (c, 1 in H_2O)

>>Derivative: *N*-Formyl

Melting Point: Mp 126° (123°)
Optical Rotation: $[\alpha]_D^{20} +24.2$ (EtOH). $[\alpha]_D^{26} +27.9$ (c, 2 in EtOH)

>>Derivative: *N*-Ac

CAS Registry Number: 20257-17-4
Melting Point: Mp 155-156°
Optical Rotation: $[\alpha]_D^{25} -5.3$ (c, 2 in H_2O). $[\alpha]_D +21.5$ (c, 2 in EtOH)

>>Derivative: *N*-Benzenesulfonyl

Melting Point: Mp 147-148°
Optical Rotation: $[\alpha]_D^{20} +30.7$ (EtOH)

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

CAS Registry Number: 73-32-5

Molecular Formula: $C_6H_{13}NO_2$
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: $[\alpha]_D +16.3$ (H_2O). $[\alpha]_D +51.8$ (5*M* HCl)
Solubility: Mod. sol. H_2O (4.12 g/100 g at 25°)
pKa Value: pK_{a1} 2.36; pK_{a2} 9.68 (NH_2)
Other Data: Isoelectric point 6.02. Bitter taste

Aldrich: 15171-8
Fluka: 58880
Sigma: I2752