



Optical Rotation: $[\alpha]_D^{22} -44.1$ (c, 1 in 6M HCl)

>> **Variant:** (2*S*,3*R*)-form

Synonym(s): L-*threo*-form. Alloisoleucine

CAS Registry Number: 1509-34-8

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%

Melting Point: Mp 278 dec.°

Optical Rotation: $[\alpha]_D^{25} +15.7$ (c, 2 in H₂O). $[\alpha]_D^{25} +34.9$ (c, 4 in 4M HCl). $[\alpha]_D +40.5$ (c, 1 in 5M HCl)

pKa Value: p*K*_{a1} 2.32; p*K*_{a2} 9.76 (25°)

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: $[\alpha]_D^{25} +15$ (c, 1 in H₂O)

>> **Derivative:** Amide; hydrochloride

CAS Registry Number: 63328-67-6

Melting Point: Mp 240-241 dec.°

Optical Rotation: $[\alpha]_D^{25} +32$ (c, 1 in H₂O)

>> **Derivative:** N-Formyl

Melting Point: Mp 126° (123°)

Optical Rotation: $[\alpha]$ +27.9 (c, 2 in EtOH)