



CAS Registry Number: 50816-94-9

Molecular Formula: C₉H₁₉NO₂

Molecular Weight: 173.255

Accurate Mass: 173.141579

Percentage Composition: C 62.39%; H 11.05%; N 8.08%; O 18.47%

Biological Source: Isol. from Cannabis seeds

Physical Description: Noncryst.

Optical Rotation: [α]_D²⁰ +18 (c, 1 in CHCl₃)

>> **Variant:** (2*RS*,3*RS*)-form

Synonym(s): (±)-*erythro*-form. (±)-Isoleucine. FEMA 3295

CAS Registry Number: 443-79-8

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%

Use/Importance: Dietary supplement, nutrient

Physical Description: Cryst. (EtOH)

Melting Point: Mp 275° (sealed tube)

Solubility: Sl. sol. H₂O

pKa Value: p*K*_{a1} 2.66; p*K*_{a2} 9.7 (25°, 0.5*M* KCl)

Aldrich: 29868-9

Fluka: 58885

Sigma: I2627

>> **Derivative:** *N*-Formyl

CAS Registry Number: 4101-35-3

Melting Point: Mp 121°

>> **Derivative:** *N*-Ac

CAS Registry Number: 73465-39-1

Melting Point: Mp 117-123°

>> **Derivative:** *N*-(4-Methylbenzenesulfonyl)

Melting Point: Mp 139-140°

>> **Variant:** (2*RS*,3*SR*)-form

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

CAS Registry Number: 3107-04-8

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%

Fluka: 5706

>> **Derivative:** Et ester

Boiling Point: Bp₁₅ 85-88°

>> **Derivative:** *N*-Ac

CAS Registry Number: 33601-90-0

Melting Point: Mp 168°

References: