



>>Derivative: *N*-Me

Synonym(s): *N*-Methylisoleucine

CAS Registry Number: 4125-98-8

Molecular Formula: $C_7H_{15}NO_2$

Molecular Weight: 145.201

Accurate Mass: 145.110279

Percentage Composition: C 57.90%; H 10.41%; N 9.65%; O 22.04%

Phaseolus vulgaris

Melting Point: Mp 290-291°

Optical Rotation: $[\alpha]_D^{26} +27.5$ (c, 1.07 in H_2O). $[\alpha]_D +47.7$ (c, 1.06 in 6*M* HCl)

>>Derivative: *N*-Tri-Me, betaine

CAS Registry Number: 50816-94-9

Molecular Formula: $C_9H_{19}NO_2$

Molecular Weight: 173.255

Accurate Mass: 173.141579

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

Physical Description: Noncryst.

Optical Rotation: $[\alpha]_D^{20} +18$ (c, 1 in $CHCl_3$)

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

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

CAS Registry Number: 443-79-8

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%

Use/Importance: Dietary supplement, nutrient

Physical Description: Cryst. (EtOH)

Melting Point: Mp 275° (sealed tube)

Solubility: Sl. sol. H_2O

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

Aldrich: 29868-9

Fluka: 58885

Sigma: I2627