Molecular Weight: 271.337
Accurate Mass: 271.087829
Percentage Composition: C 53.12%; H 6.31%; N 5.16%; O 23.59%; S 11.82%
Melting Point: Mp 153-154°
Optical Rotation: $[\alpha]_D^{20}$+14.3 (NaOH). $[\alpha]_D$ –25.5 (EtOH)

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

Molecular Formula: $C_{13}H_{19}NO_4S$
Molecular Weight: 285.363
Accurate Mass: 285.103479
Percentage Composition: C 54.72%; H 6.71%; N 4.91%; O 22.43%; S 11.24%
Melting Point: Mp 130-132°

>>**Derivative:** *N*-Me

CAS Registry Number: 39554-61-5
Melting Point: Mp 290-291°
Optical Rotation: $[\alpha]_D^{20}$–31 (c, 1 in H_2O)

>>**Variant:** (2*R*,3*S*)-form
Synonym(s): D-*threo*-form. D-Alloisoleucine
CAS Registry Number: 1509-35-9
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%
Melting Point: Mp 274-275 dec.°
Optical Rotation: $[\alpha]_D^{25}$–15.6 (c, 2 in H_2O). $[\alpha]_D$ –38.4 (c, 4 in 6*M* HCl)
pKa Value: pK_{a1} 2.2; pK_{a2} 9.62 (25°, H_2O)

Fluka: 5705
Sigma: I0380

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

Melting Point: Mp 126°
Optical Rotation: $[\alpha]_D^{20}$–25.2 (EtOH)

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

CAS Registry Number: 54831-20-8
Melting Point: Mp 156°
Optical Rotation: $[\alpha]_D^{25}$–21.5 (c, 2 in EtOH)
Sigma: A0501

>>**Derivative:** *N*-Benzenesulfonyl

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

>>**Derivative:** *N*-Me

CAS Registry Number: 50673-48-8
Melting Point: Mp 288-290°
Optical Rotation: $[\alpha]_D^{22}$–44.1 (c, 1 in 6*M* HCl)

>>**Variant:** (2*S*,3*R*)-form
Synonym(s): L-*threo*-form. Alloisoleucine

CAS Registry Number: 1509-34-8
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%
Melting Point: Mp 278 dec.°