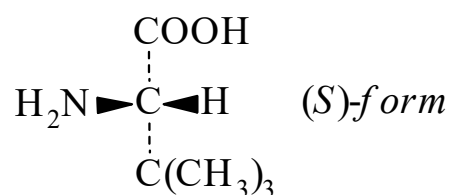




>>Entry Name: 2-Amino-3,3-dimethylbutanoic acid

Synonym(s): 3-Methylvaline, 9Cl. *tert*-Butylglycine. *tert*-Leucine. 2-Aminoneohexanoic acid. Bug. Pseudoleucine. ψ -Leucine



CAS Registry Number: 471-50-1

Related CAS Registry Numbers(s): 75158-12-2

Molecular Formula: $\text{C}_6\text{H}_{13}\text{NO}_2$

Molecular Weight: 131.174

Accurate Mass: 131.094629

Percentage Composition: C 54.94%; H 9.99%; N 10.68%; O 24.39%

>>Variant: (*R*)-form

Molecular Formula: $\text{C}_6\text{H}_{13}\text{NO}_2$

Molecular Weight: 131.174

Accurate Mass: 131.094629

Percentage Composition: C 54.94%; H 9.99%; N 10.68%; O 24.39%

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 61169-85-5

Molecular Formula: $\text{C}_{10}\text{H}_{21}\text{NO}_2$

Molecular Weight: 187.281

Accurate Mass: 187.157229

Percentage Composition: C 64.13%; H 11.30%; N 7.48%; O 17.09%

Melting Point: Mp 157.5-158.5° (as acid oxalate)

Boiling Point: Bp₂₁ 90-91°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -1.57$ (neat) (93.5% op)

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 20859-02-3

Molecular Formula: $\text{C}_6\text{H}_{13}\text{NO}_2$

Molecular Weight: 131.174

Accurate Mass: 131.094629

Percentage Composition: C 54.94%; H 9.99%; N 10.68%; O 24.39%

Biological Source: Residue from Bottromycin [GQN88-M](#)

Use/Importance: Chiral inducer in asymmetric syntheses. Leucine analogue in modified peptides

Melting Point: Mp 248 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -9.5$ (c, 3 in H_2O). $[\alpha]_{\text{D}}^{25} +8.7$ (c, 3 in 5M HCl)

Other Data: Varying optical rotations have been reported

Aldrich: 26910-7

Fluka: 61825

Sigma: B9013

Other: Chiroscience

>>Derivative: Me ester

CAS Registry Number: 63038-26-6

Molecular Formula: $\text{C}_7\text{H}_{15}\text{NO}_2$

Molecular Weight: 145.201

Accurate Mass: 145.110279

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

Melting Point: Mp 170°

Optical Rotation: $[\alpha]_{\text{D}}^{23} +17$ (c, 1 in MeOH)

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 31556-74-8

Boiling Point: Bp₁₈ 87-89°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +1.55$ (neat) (92.3% op)