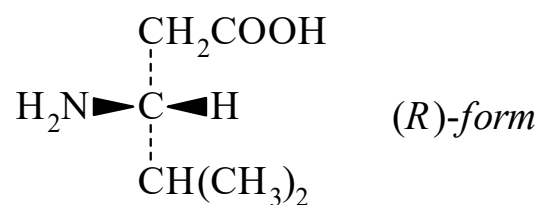




>>Entry Name: 3-Amino-4-methylpentanoic acid, 9CI

Synonym(s): β -Leucine. β -Aminoisocaproic acid



CAS Registry Number: 5699-54-7

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%

General Statement: Some confusion over abs. config. A recent paper gives opposite rotations to the determination of Balenovic, without comment. The assignment given here follows Balenovic. Unusually for this amino acid (R) $\equiv$ L and (S) $\equiv$ D

>>Variant: (R)-form

Synonym(s): L-form

CAS Registry Number: 75992-50-6

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%

Melting Point: Mp 201-202°

Optical Rotation: $[\alpha]_{\text{D}}$ +55.2

>>Derivative: N -9-Fluorenylmethoxycarbonyl

CAS Registry Number: 172695-33-9

Molecular Formula: $\text{C}_{21}\text{H}_{23}\text{NO}_4$

Molecular Weight: 353.417

Accurate Mass: 353.162709

Percentage Composition: C 71.37%; H 6.56%; N 3.96%; O 18.11%

Physical Description: Crys. ($\text{CHCl}_3/\text{MeOH}$)

Melting Point: Mp 158°

Optical Rotation: $[\alpha]_{\text{D}}^{25}$ -21.5 (c, 0.465 in CHCl_3)

>>Derivative: N -9-Fluorenylmethoxycarbonyl, Me ester

CAS Registry Number: 193954-34-6

Molecular Formula: $\text{C}_{22}\text{H}_{25}\text{NO}_4$

Molecular Weight: 367.444

Accurate Mass: 367.178359

Percentage Composition: C 71.91%; H 6.86%; N 3.81%; O 17.42%

Physical Description: Cryst.

Melting Point: Mp 70-72°

Optical Rotation: $[\alpha]_{\text{D}}$ -26 (c, 0.65 in CHCl_3)

>>Variant: (S)-form

Synonym(s): D-form

CAS Registry Number: 40469-85-0

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%

Melting Point: Mp 197-200°

Optical Rotation: $[\alpha]_{\text{D}}^{24}$ -39.2 (c, 0.51 in H_2O). $[\alpha]_{\text{D}}^{20}$ -23.9 (c, 0.88 in 1M HCl). $[\alpha]_{\text{D}}^{20}$ +4.6 (c, 0.65 in 1M NaOH)

>>Derivative: Et ester

Molecular Formula: $\text{C}_8\text{H}_{17}\text{NO}_2$

Molecular Weight: 159.228

Accurate Mass: 159.125929

Percentage Composition: C 60.35%; H 10.76%; N 8.80%; O 20.10%

Physical Description: Oil

Optical Rotation: $[\alpha]$