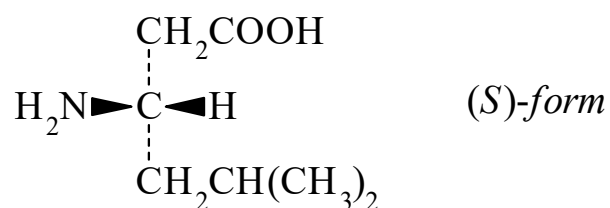




>>Entry Name: 3-Amino-5-methylhexanoic acid, 9CI

Synonym(s):  $\beta$ -Homoleucine



CAS Registry Number: 3653-34-7

Related CAS Registry Numbers(s): 96386-92-4

Extra CAS Registry Numbers(s): 91298-67-8

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%

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 22818-43-5

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%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 225° (215-216°)

Optical Rotation:  $[\alpha]_D +28$  (c, 3 in  $H_2O$ ).  $[\alpha]_D +38.4$  (c, 0.54 in  $H_2O$ )

>>Derivative: *N*-Ac, Me ester

CAS Registry Number: 136744-89-3

Molecular Formula:  $C_{10}H_{19}NO_3$

Molecular Weight: 201.265

Accurate Mass: 201.136494

Percentage Composition: C 59.68%; H 9.51%; N 6.96%; O 23.85%

Optical Rotation:  $[\alpha]_D^{25} -42$  (c, 1.06 in  $CHCl_3$ )

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

CAS Registry Number: 22818-42-4

Physical Description: Cryst. ( $Et_2O$ /petrol)

Melting Point: Mp 109.5-111°

>>Derivative: *N*-(9-Fluorenylmethoxycarbonyl)

CAS Registry Number: 193887-44-4

Molecular Formula:  $C_{22}H_{25}NO_4$

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. ( $CHCl_3$ /hexane)

Melting Point: Mp 108-110°

Optical Rotation:  $[\alpha]_D -22.2$  (c, 1.12 in  $CHCl_3$ )

>>Derivative: *N*-(9-Fluorenylmethoxycarbonyl), Me ester

CAS Registry Number: 193954-35-7

Molecular Formula:  $C_{23}H_{27}NO_4$

Molecular Weight: 381.471

Accurate Mass: 381.194009

Percentage Composition: C 72.42%; H 7.13%; N 3.67%; O 16.78%

Physical Description: Cryst.

Melting Point: Mp 74-76°

Optical Rotation:  $[\alpha]_D -34$  (c, 0.85 in  $CHCl_3$ )