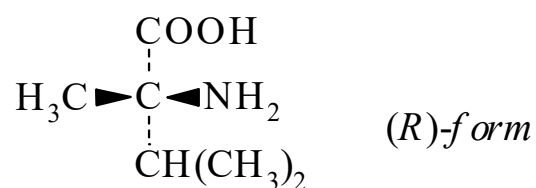




>>Entry Name: 2-Amino-2,3-dimethylbutanoic acid

Synonym(s): 2-Methylvaline, 8Cl. 3-Methylisovaline, 9Cl



CAS Registry Number: 4378-19-2

Related CAS Registry Numbers(s): 90376-97-9 90376-99-1 92487-58-6

Molecular Formula: C₆H₁₃NO₂

Molecular Weight: 131.174

Accurate Mass: 131.094629

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

Use/Importance: Strong Type I/III β-turn and helix former in peptides

>>Variant: (R)-form

Synonym(s): D-form

CAS Registry Number: 53940-82-2

Molecular Formula: C₆H₁₃NO₂

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 215 dec.°

Optical Rotation: [α]_D +3.9 (c, 1.3 in H₂O)

>>Derivative: Me ester

CAS Registry Number: 71785-68-7

Molecular Formula: C₇H₁₅NO₂

Molecular Weight: 145.201

Accurate Mass: 145.110279

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

Boiling Point: Bp₅ 45-55° (lit. gives a pressure range)

>>Derivative: Amide

CAS Registry Number: 90376-98-0

Molecular Formula: C₆H₁₄N₂O

Molecular Weight: 130.189

Accurate Mass: 130.110613

Percentage Composition: C 55.35%; H 10.84%; N 21.52%; O 12.29%

Melting Point: Mp 73.5-78.5°

>>Derivative: N-Trifluoroacetyl

CAS Registry Number: 53940-87-7

Molecular Formula: C₈H₁₂F₃NO₃

Molecular Weight: 227.183

Accurate Mass: 227.076928

Percentage Composition: C 42.30%; H 5.32%; F 25.09%; N 6.17%; O 21.13%

Optical Rotation: [α]₄₀₀²⁵ -18.6 (c, 1.5 in EtOH)

>>Derivative: N-Benzoyl; Me ester

CAS Registry Number: 169566-74-9

Molecular Formula: C₁₄H₁₉NO₃

Molecular Weight: 249.309

Accurate Mass: 249.136494

Percentage Composition: C 67.45%; H 7.68%; N 5.62%; O 19.25%

Physical Description: Oil

Optical Rotation: [α]_D -20.5 (c, 0.2 in CHCl₃)