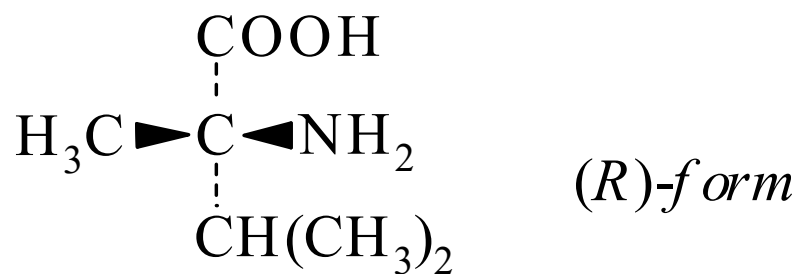




>>Entry Name: 2-Amino-2,3-dimethylbutanoic acid

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

Molecular Weight: 131.174

Accurate Mass: 131.094629

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

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

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 215 dec. $^\circ$

Optical Rotation: $[\alpha]_{\text{D}} +3.9$ (c, 1.3 in H_2O)

>>Derivative: Me ester

CAS Registry Number: 71785-68-7

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%

Boiling Point: Bp₅ 45-55 $^\circ$ (lit. gives a pressure range)

>>Derivative: Amide

CAS Registry Number: 90376-98-0

Molecular Formula: $\text{C}_6\text{H}_{14}\text{N}_2\text{O}$

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 $^\circ$

>>Derivative: N-Trifluoroacetyl

CAS Registry Number: 53940-87-7

Molecular Formula: $\text{C}_8\text{H}_{12}\text{F}_3\text{NO}_3$

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: $[\alpha]_{400}^{25} -18.6$ (c, 1.5 in EtOH)

>>Derivative: N-Benzoyl; Me ester

CAS Registry Number: 169566-74-9

Molecular Formula: $\text{C}_{14}\text{H}_{19}\text{NO}_3$

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: $[\alpha]_{\text{D}} -20.5$ (c, 0.2 in CHCl_3)