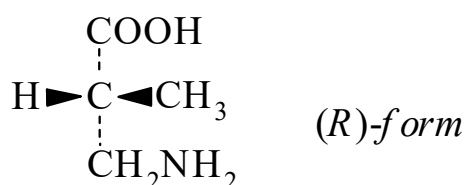




>>Entry Name: 3-Amino-2-methylpropanoic acid, 9CI

Synonym(s): α -Methyl- β -alanine. 3-Aminoisobutyric acid. β -Aminoisobutyric acid



CAS Registry Number: 144-90-1

Related CAS Registry Numbers(s): 16948-10-0

Molecular Formula: $\text{C}_4\text{H}_9\text{NO}_2$

Molecular Weight: 103.121

Accurate Mass: 103.063329

Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%

>>Variant: (R)-form

CAS Registry Number: 2140-95-6

Molecular Formula: $\text{C}_4\text{H}_9\text{NO}_2$

Molecular Weight: 103.121

Accurate Mass: 103.063329

Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%

Biological Source: Present in iris (*Iris tingitana*) bulbs and in human urine. Also from seeds of *Lunaria annua*

Physical Description: Cryst. (EtOH)

Melting Point: Mp 183°

Optical Rotation: $[\alpha]_{\text{D}}^{26} -21$ (c, 0.43 in H_2O)

>>Derivative: *N*-*tert*-Butyloxycarbonyl

CAS Registry Number: 132696-45-8

Molecular Formula: $\text{C}_9\text{H}_{17}\text{NO}_4$

Molecular Weight: 203.238

Accurate Mass: 203.115759

Percentage Composition: C 53.19%; H 8.43%; N 6.89%; O 31.49%

Physical Description: Cryst. (Et_2O)

Melting Point: Mp 69.5-70.5°

Optical Rotation: $[\alpha]_{\text{D}} -18.4$ (c, 2 in MeOH)

>>Variant: (S)-form

CAS Registry Number: 4249-19-8

Molecular Formula: $\text{C}_4\text{H}_9\text{NO}_2$

Molecular Weight: 103.121

Accurate Mass: 103.063329

Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%

Physical Description: Cryst.

Melting Point: Mp 184-186°

Optical Rotation: $[\alpha]_{\text{D}} -21$ (c, 0.43 in H_2O)

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

CAS Registry Number: 203854-58-4

Extra CAS Registry Numbers(s): 161125-39-9 186320-19-4

Molecular Formula: $\text{C}_{19}\text{H}_{19}\text{NO}_4$

Molecular Weight: 325.363

Accurate Mass: 325.131409

Percentage Composition: C 70.14%; H 5.89%; N 4.30%; O 19.67%

Physical Description: Cryst. (CHCl_3 /hexane)

Melting Point: Mp 162-163°

Optical Rotation: $[\alpha]_{\text{D}} +9.6$ (c, 1.0 in CHCl_3)