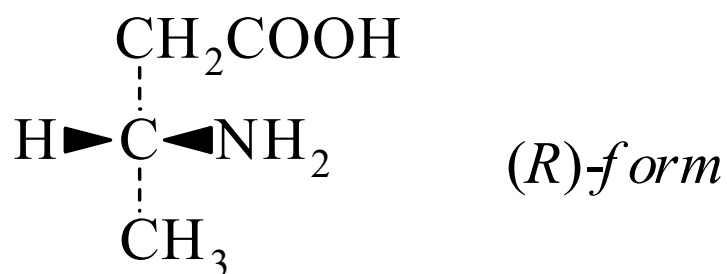




>>Entry Name: 3-Aminobutanoic acid, 9CI

Synonym(s): β -Homoalanine



CAS Registry Number: 541-48-0

Extra CAS Registry Numbers(s): 28805-76-7

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: Prod. by *Oryza sativa*, *Pinellia ternata* and *Myrothecium verrucaria* (no opt. rotns. reported)

>>Variant: (*R*)-form

CAS Registry Number: 3775-73-3

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: Prisms (MeOH)

Melting Point: Mp 218-219°

Optical Rotation: $[\alpha]_{\text{D}}^{23} -39$ (c, 0.4 in H_2O) (op)

>>Derivative: Me ester

CAS Registry Number: 103189-63-5

Molecular Formula: $\text{C}_5\text{H}_{11}\text{NO}_2$

Molecular Weight: 117.147

Accurate Mass: 117.078979

Percentage Composition: C 51.26%; H 9.46%; N 11.96%; O 27.31%

Boiling Point: Bp₁₁ 54-55°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -32$ (c, 1 in EtOH)

>>Derivative: Et ester

CAS Registry Number: 115880-49-4

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%

Physical Description: Yellow glass (as hydrochloride)

Optical Rotation: $[\alpha]_{\text{D}}^{23} -19$ (c, 0.6 in H_2O)

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

CAS Registry Number: 121054-32-8

Molecular Formula: $\text{C}_{12}\text{H}_{15}\text{NO}_3$

Molecular Weight: 221.255

Accurate Mass: 221.105194

Percentage Composition: C 65.14%; H 6.83%; N 6.33%; O 21.69%

Melting Point: Mp 108-109°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +40.3$ (c, 0.81 in CHCl_3)