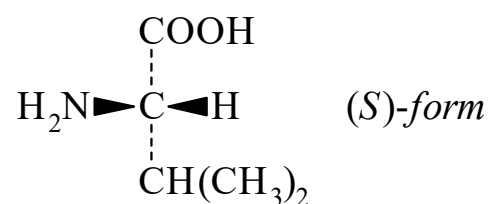




>>Entry Name: Valine

ENTRY UNDER REVIEW

Synonym(s): 2-Amino-3-methylbutanoic acid, 9Cl. 2-Aminoisovaleric acid. Val



CAS Registry Number: 7004-03-7

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%

>>Variant: (R)-form

Synonym(s): D-form

CAS Registry Number: 640-68-6

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%

Biological Source: Residue present in microbial cell walls and in antibiotics, e.g. actinomycins

Physical Description: Plates (EtOH aq.)

Melting Point: Mp 156-157.5° (293° dec. sealed tube)

Optical Rotation: $[\alpha]_{\text{D}}^{25} -6.1$ (H_2O). $[\alpha]_{\text{D}}^{20} -28.8$ (c, 1 in 5M HCl) (100% op)

Solubility: Sol. H_2O

Aldrich: 85598-7

Fluka: 94630

Sigma: V0250

>>Derivative: Me ester

CAS Registry Number: 21685-47-2

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%

Physical Description: Liq.

>>Derivative: Me ester; hydrochloride

CAS Registry Number: 7146-15-8

Physical Description: Plates (MeOH/Et₂O)

Melting Point: Mp 167.5-168°

Optical Rotation: $[\alpha]_{\text{D}}^{21} -15.6$ (c, 2 in H_2O)

Fluka: 94665

>>Derivative: Amide

CAS Registry Number: 133170-58-8

Molecular Formula: $\text{C}_5\text{H}_{12}\text{N}_2\text{O}$

Molecular Weight: 116.163

Accurate Mass: 116.094963

Percentage Composition: C 51.70%; H 10.41%; N 24.12%; O 13.77%

Melting Point: Mp 268-269 dec.° (as hydrochloride)

Optical Rotation: $[\alpha]_{\text{D}}^{24} -28.3$ (c, 1 in H_2O)