



>>Entry Name: *N*-Alanylglycine

$\text{H}_3\text{CCH}(\text{NH}_2)\text{CONHCH}_2\text{COOH}$

Molecular Formula: $\text{C}_5\text{H}_{10}\text{N}_2\text{O}_3$

Molecular Weight: 146.146

Accurate Mass: 146.069143

Percentage Composition: C 41.09%; H 6.90%; N 19.17%; O 32.84%

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 3997-90-8

Molecular Formula: $\text{C}_5\text{H}_{10}\text{N}_2\text{O}_3$

Molecular Weight: 146.146

Accurate Mass: 146.069143

Percentage Composition: C 41.09%; H 6.90%; N 19.17%; O 32.84%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 233-235°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -46.6$ (c, 1.02 in H_2O)

Sigma: A0628

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 687-69-4

Molecular Formula: $\text{C}_5\text{H}_{10}\text{N}_2\text{O}_3$

Molecular Weight: 146.146

Accurate Mass: 146.069143

Percentage Composition: C 41.09%; H 6.90%; N 19.17%; O 32.84%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 230-231.5 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{21} +50.9$ (c, 2.0 in H_2O)

Fluka: 5270

Rare Chemicals Library: S45504-0

Sigma: A0878

>>Derivative: *N*-Benzyloxycarbonyl

CAS Registry Number: 3235-17-4

Molecular Formula: $\text{C}_{13}\text{H}_{18}\text{N}_2\text{O}_5$

Molecular Weight: 282.296

Accurate Mass: 282.121573

Percentage Composition: C 55.31%; H 6.43%; N 9.92%; O 28.34%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 134-135°

Optical Rotation: $[\alpha]_{\text{D}}^{23} -17.3$ (c, 2.0 in EtOH)

>>Derivative: *N*-Benzyloxycarbonyl, Et ester

CAS Registry Number: 2503-32-4

Molecular Formula: $\text{C}_{15}\text{H}_{22}\text{N}_2\text{O}_5$

Molecular Weight: 310.349

Accurate Mass: 310.152873

Percentage Composition: C 58.05%; H 7.14%; N 9.03%; O 25.78%

Physical Description: Cryst. (EtOAc/cyclohexane)

Melting Point: Mp 88-89.5°

Optical Rotation: $[\alpha]_{\text{D}}^{19} -18.3$ (c, 2.0 in EtOH)

>>Variant: ($\pm$)-form

CAS Registry Number: 1188-01-8

Molecular Formula: $\text{C}_5\text{H}_{10}\text{N}_2\text{O}_3$

Molecular Weight: 146.146

Accurate Mass: 146.069143

Percentage Composition: C 41.09%; H 6.90%; N 19.17%; O 32.84%

pKa Value: $\text{pK}_{\text{a}2}$ 8.18 (25°, 0.1M NaCl)

Sigma: A0753