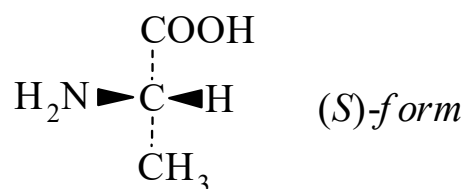




>>Entry Name: Alanine, INN, USAN

Synonym(s): 2-Aminopropanoic acid, 9CI. α -Alanine. Ala



Related CAS Registry Numbers(s): 2134-48-7 2491-20-5 3082-75-5 17831-01-5 33208-99-0 34404-37-0 95596-57-9 98204-12-7

Molecular Formula: $\text{C}_3\text{H}_7\text{NO}_2$

Molecular Weight: 89.094

Accurate Mass: 89.047679

Percentage Composition: C 40.44%; H 7.92%; N 15.72%; O 35.92%

>>Variant: (R)-form

Synonym(s): D-form

CAS Registry Number: 338-69-2

Molecular Formula: $\text{C}_3\text{H}_7\text{NO}_2$

Molecular Weight: 89.094

Accurate Mass: 89.047679

Percentage Composition: C 40.44%; H 7.92%; N 15.72%; O 35.92%

Biological Source: Occurs in the cell walls of bacteria and in some higher plants

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 295-297 dec. $^\circ$

Optical Rotation: $[\alpha]_{\text{D}}^{25} -1.8$ (c, 1 in H_2O). $[\alpha]_{\text{D}} -14.6$ (c, 1 in 5M HCl)

Solubility: Sol. hot H_2O

Aldrich: 16265-5

Fluka: 5140

Sigma: A7377

>>Derivative: Hydrochloride

Optical Rotation: $[\alpha]_{\text{D}}^{20} -10.3$ (H_2O)

Solubility: Sol. H_2O

>>Derivative: Me ester

CAS Registry Number: 21705-13-5

Extra CAS Registry Numbers(s): 14316-06-4

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%

Melting Point: Mp 109-111 $^\circ$ (as hydrochloride)

>>Derivative: Et ester

CAS Registry Number: 30959-96-7

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%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 104-105 $^\circ$

Optical Rotation: $[\alpha]_{\text{D}}^{20} +6.91$ (EtOH)

>>Derivative: Benzyl ester

CAS Registry Number: 17831-02-6

Molecular Formula: $\text{C}_{10}\text{H}_{13}\text{NO}_2$

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Melting Point: Mp 139-140 $^\circ$ (as hydrochloride)

Optical Rotation: $[\alpha]_{\text{D}}^{25} +10.5$ (c, 2 in 0.1M HCl)