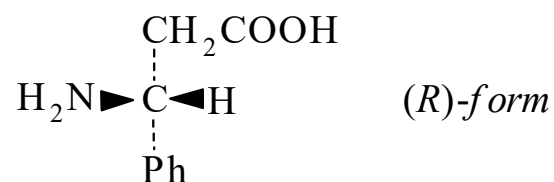




>>Entry Name: 3-Amino-3-phenylpropanoic acid

Synonym(s): β -Aminobenzenepropanoic acid, 9Cl. β -Aminohydrocinnamic acid. β -Phenyl- β -alanine



CAS Registry Number: 614-19-7

Molecular Formula: $\text{C}_9\text{H}_{11}\text{NO}_2$

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Aldrich: 15949-2

Rare Chemicals Library: S1461-4

>>Variant: (*R*)-form

CAS Registry Number: 13921-90-9

Molecular Formula: $\text{C}_9\text{H}_{11}\text{NO}_2$

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Physical Description: Plates (H_2O)

Melting Point: Mp *ca.* 234-235°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +7$ (H_2O)

>>Derivative: Et ester

Molecular Formula: $\text{C}_{11}\text{H}_{15}\text{NO}_2$

Molecular Weight: 193.245

Accurate Mass: 193.110279

Percentage Composition: C 68.37%; H 7.82%; N 7.25%; O 16.56%

Boiling Point: Bp_{13} 155°

Optical Rotation: $[\alpha]_{\text{D}}^{24} +13.7$

>>Derivative: Et ester; hydrochloride

Melting Point: Mp 137-147°

>>Derivative: *N*-Formyl

Molecular Formula: $\text{C}_{10}\text{H}_{11}\text{NO}_3$

Molecular Weight: 193.202

Accurate Mass: 193.073894

Percentage Composition: C 62.17%; H 5.74%; N 7.25%; O 24.84%

Physical Description: Needles (H_2O)

Melting Point: Mp 142-143°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +116.4$ (EtOH)

>>Derivative: *N,N*-Di-Me

Synonym(s): 3-(Dimethylamino)-3-phenylpropanoic acid. Winterstein's acid

CAS Registry Number: 94099-69-1

Molecular Formula: $\text{C}_{11}\text{H}_{15}\text{NO}_2$

Molecular Weight: 193.245

Accurate Mass: 193.110279

Percentage Composition: C 68.37%; H 7.82%; N 7.25%; O 16.56%

>>Derivative: *N,N*-Di-Me, Et ester

Molecular Formula: $\text{C}_{13}\text{H}_{19}\text{NO}_2$

Molecular Weight: 221.299

Accurate Mass: 221.141579

Percentage Composition: C 70.56%; H 8.65%; N 6.33%; O 14.46%

Physical Description: Oil

Optical Rotation: $[\alpha]$