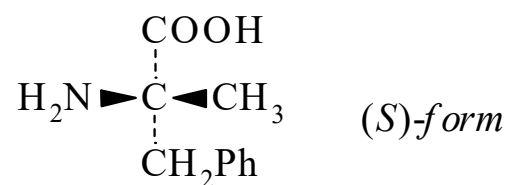




>>Entry Name: 2-Amino-2-methyl-3-phenylpropanoic acid

Synonym(s): α -Methylphenylalanine, 9Cl. 2-Methyl-3-phenylalanine, 8Cl. 2-Amino-2-phenylisobutyric acid



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%

>>Variant: (R)-form

CAS Registry Number: 17350-84-4

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%

Optical Rotation: $[\alpha]_{\text{D}} +20$ (c, 0.11 in MeOH)

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 23239-35-2

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%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 308-309 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{22} -22$ (c, 1 in H_2O)

>>Derivative: Hydrochloride

CAS Registry Number: 30990-90-0

Melting Point: Mp 249 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -8.6$ (c, 1 in H_2O)

>>Derivative: Me ester

CAS Registry Number: 28385-45-7

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: $\text{Bp}_{0.01} 90^\circ$

Optical Rotation: $[\alpha]_{\text{D}}^{20} +2.4$ (c, 0.8 in EtOH)

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

CAS Registry Number: 1132-26-9

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%

Physical Description: Needles (H_2O)

Melting Point: Mp 294-295 dec.°

Solubility: Sol. AcOH; insol. most org. solvs.

Aldrich: 28665-6

Fluka: 68627

Sigma: M3635

>>Derivative: Hydrochloride

Other Data: Dec. at 236°