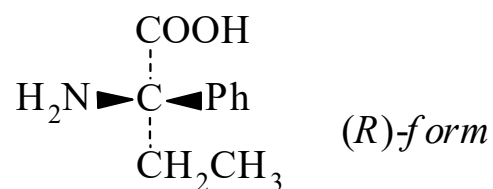




>>Entry Name: 2-Amino-2-phenylbutanoic acid

Synonym(s): α -Amino- α -ethylbenzeneacetic acid, 9CI



CAS Registry Number: 5438-07-3

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: 33875-38-6

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 250-255°

Optical Rotation: $[\alpha]_{\text{D}} -41$

>>Variant: (S)-form

CAS Registry Number: 52247-77-5

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. (EtOH aq.)

Melting Point: Mp 255-265 dec., 270°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +34.4$ (c, 1.63 in H_2O)

>>Derivative: Me ester

CAS Registry Number: 52165-71-6

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%

Physical Description: Oil

Boiling Point: $\text{Bp}_{1.5}$ 85-87°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +10$ (c, 1.02 in EtOH)

>>Derivative: Et ester

CAS Registry Number: 52165-63-6

Molecular Formula: $\text{C}_{12}\text{H}_{17}\text{NO}_2$

Molecular Weight: 207.272

Accurate Mass: 207.125929

Percentage Composition: C 69.54%; H 8.27%; N 6.76%; O 15.44%

Physical Description: Oil

Boiling Point: Bp_3 90-91°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +14.6$ (c, 1.08 in EtOH)

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

CAS Registry Number: 20318-28-9

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: Prisms or needles (H_2O contg. NH_3)

Melting Point: Mp 275 dec.°

Solubility: Sol. AcOH, insol. most other solvs.