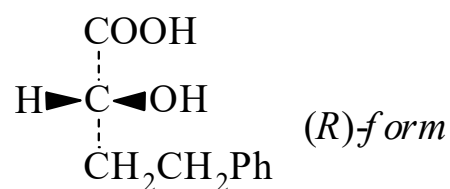




>>Entry Name: 2-Hydroxy-4-phenylbutanoic acid

Synonym(s): α -Hydroxybenzenebutanoic acid, 9CI. 3-Benzylactic acid



CAS Registry Number: 4263-93-8

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{O}_3$

Molecular Weight: 180.203

Accurate Mass: 180.078645

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

>>Variant: (R)-form

CAS Registry Number: 29678-81-7

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{O}_3$

Molecular Weight: 180.203

Accurate Mass: 180.078645

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

Melting Point: Mp 114 subl.°

Optical Rotation: $[\alpha]_{\text{D}} +12.9$

Aldrich: 42008-5

Fluka: 56112

Other: Kaneka I-3

>>Derivative: Et ester

CAS Registry Number: 90315-82-5

Molecular Formula: $\text{C}_{12}\text{H}_{16}\text{O}_3$

Molecular Weight: 208.257

Accurate Mass: 208.109945

Percentage Composition: C 69.21%; H 7.74%; O 23.05%

Physical Description: Liq.

Boiling Point: Bp₁ 120°

Optical Rotation: $[\alpha]_{\text{D}}^{23} -20.8$ (c, 1.0 in CHCl_3) (94% ee). $[\alpha]_{\text{D}}^{20} -21.7$

Aldrich: 46082-6

Fluka: 56114

>>Derivative: Amide

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 124°

Optical Rotation: $[\alpha]_{\text{D}}^{21} +35.2$ (EtOH)

>>Variant: (S)-form

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{O}_3$

Molecular Weight: 180.203

Accurate Mass: 180.078645

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

Melting Point: Mp 114-116°

Optical Rotation: $[\alpha]_{\text{D}}^{27} -9.9$

>>Derivative: Me ester

CAS Registry Number: 68844-69-9

Molecular Formula: $\text{C}_{11}\text{H}_{14}\text{O}_3$

Molecular Weight: 194.23

Accurate Mass: 194.094295

Percentage Composition: C 68.02%; H 7.26%; O 24.71%

Physical Description: Oil

Boiling Point: Bp₁₁ 142-143°

Optical Rotation: $[\alpha] \quad \quad \quad -22.3$ (H_2O)