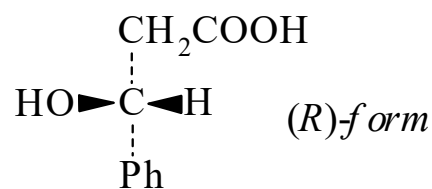




>>Entry Name: 3-Hydroxy-3-phenylpropanoic acid

Synonym(s): β -Hydroxybenzenepropanoic acid, 9Cl. 3-Phenylhydracrylic acid, 8Cl. β -Hydroxyhydrocinnamic acid



CAS Registry Number: 3480-87-3

Molecular Formula: $\text{C}_9\text{H}_{10}\text{O}_3$

Molecular Weight: 166.176

Accurate Mass: 166.062995

Percentage Composition: C 65.05%; H 6.07%; O 28.88%

Biological Source: Isol. from *Lobelia inflata*

>>Variant: (R)-form

CAS Registry Number: 2768-42-5

Molecular Formula: $\text{C}_9\text{H}_{10}\text{O}_3$

Molecular Weight: 166.176

Accurate Mass: 166.062995

Percentage Composition: C 65.05%; H 6.07%; O 28.88%

Melting Point: Mp 115-116°

Optical Rotation: $[\alpha]_{\text{D}}^{18} +19.2$ (EtOH)

>>Derivative: Ac

Melting Point: Mp 93°

Optical Rotation: $[\alpha]_{\text{D}}^{18} +63.8$

>>Derivative: Me ester

CAS Registry Number: 58692-70-9

Optical Rotation: $[\alpha]_{\text{D}} +14.1$ (EtOH)

>>Derivative: Amide

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%

Melting Point: Mp 105-106°

Optical Rotation: $[\alpha]_{\text{D}}^{13} +38.4$ (EtOH)

>>Variant: (S)-form

CAS Registry Number: 36567-72-3

Molecular Formula: $\text{C}_9\text{H}_{10}\text{O}_3$

Molecular Weight: 166.176

Accurate Mass: 166.062995

Percentage Composition: C 65.05%; H 6.07%; O 28.88%

Melting Point: Mp 115-116°

Optical Rotation: $[\alpha]_{\text{D}} -18.9$ (EtOH)

>>Derivative: Me ester

CAS Registry Number: 36615-45-9

Optical Rotation: $[\alpha]_{\text{D}} -17$ (EtOH)

>>Derivative: Ethylamide

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%

Melting Point: Mp 108-109°

Optical Rotation: $[\alpha]$