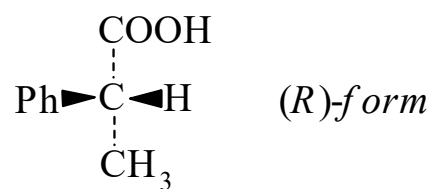




>>Entry Name: 2-Phenylpropanoic acid

Synonym(s): α -Methylbenzeneacetic acid, 9CI. Hydratropic acid, 8CI



CAS Registry Number: 492-37-5

Related CAS Registry Numbers(s): 25145-43-1 36240-11-6 42412-76-0

Molecular Formula: $\text{C}_9\text{H}_{10}\text{O}_2$

Molecular Weight: 150.177

Accurate Mass: 150.06808

Percentage Composition: C 71.98%; H 6.71%; O 21.31%

Aldrich: P3170-1

Fluka: 78995

Rare Chemicals Library: S3882-3

>>Variant: (R)-form

CAS Registry Number: 7782-26-5

Molecular Formula: $\text{C}_9\text{H}_{10}\text{O}_2$

Molecular Weight: 150.177

Accurate Mass: 150.06808

Percentage Composition: C 71.98%; H 6.71%; O 21.31%

Boiling Point: Bp_6 133-135°

Optical Rotation: $[\alpha]_{\text{D}}^{21} -73.1$ (CHCl_3)

Aldrich: 27989-7

Fluka: 78990

Sigma: P3284

>>Variant: (S)-form

CAS Registry Number: 7782-24-3

Molecular Formula: $\text{C}_9\text{H}_{10}\text{O}_2$

Molecular Weight: 150.177

Accurate Mass: 150.06808

Percentage Composition: C 71.98%; H 6.71%; O 21.31%

Boiling Point: $\text{Bp}_{0.4}$ 101-103°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +81.1$ (c, 3.108 in EtOH). $[\alpha]_{\text{D}}^{22} +97$ (neat)

Aldrich: 27990-0

Fluka: 78992

Sigma: P8159

>>Derivative: Me ester

CAS Registry Number: 28645-07-0

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{O}_2$

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Boiling Point: Bp_2 60-65°

Optical Rotation: $[\alpha]_{\text{D}}^{22} +103.5$ (neat)

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

CAS Registry Number: 2328-24-7

Molecular Formula: $\text{C}_9\text{H}_{10}\text{O}_2$

Molecular Weight: 150.177

Accurate Mass: 150.06808

Percentage Composition: C 71.98%; H 6.71%; O 21.31%

Melting Point: Mp 15-16.5°

Boiling Point: Bp 264-265°. Bp_{11} 147°

pKa Value: $\text{pK}_{\text{a}1}$ 4.3 (25°)