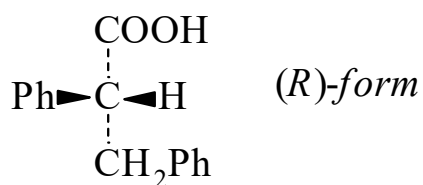




>>Entry Name: 2,3-Diphenylpropanoic acid, 8Cl

Synonym(s): α -Phenylbenzenepropanoic acid, 9Cl. Benzylphenylacetic acid. α -Phenylhydrocinnamic acid. Bibenzyl α -carboxylic acid



CAS Registry Number: 3333-15-1

Molecular Formula: $\text{C}_{15}\text{H}_{14}\text{O}_2$

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

>>Variant: (R)-form

CAS Registry Number: 17040-62-9

Molecular Formula: $\text{C}_{15}\text{H}_{14}\text{O}_2$

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

Melting Point: Mp 85-87° (82.5-84°)

Boiling Point: Bp_{0.15} 140-150°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -133.8$ (c, 0.5 in C_6H_6)

>>Variant: (S)-form

CAS Registry Number: 19041-32-8

Molecular Formula: $\text{C}_{15}\text{H}_{14}\text{O}_2$

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

Melting Point: Mp 83-84°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +140.8$ (c, 2 in C_6H_6)

>>Derivative: Et ester

CAS Registry Number: 19643-60-8

Molecular Formula: $\text{C}_{17}\text{H}_{18}\text{O}_2$

Molecular Weight: 254.328

Accurate Mass: 254.13068

Percentage Composition: C 80.28%; H 7.13%; O 12.58%

Boiling Point: Bp_{0.25} 150°

Optical Rotation: $[\alpha]_{\text{D}} +2.8$ (c, 7.5 in CHCl_3)

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

Molecular Formula: $\text{C}_{15}\text{H}_{14}\text{O}_2$

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

Melting Point: Mp 95-96° (85-87°, 82°)

Boiling Point: Bp 330-340°. Bp₂ 178-179°

>>Derivative: Me ester

CAS Registry Number: 35030-49-0

Molecular Formula: $\text{C}_{16}\text{H}_{16}\text{O}_2$

Molecular Weight: 240.301

Accurate Mass: 240.11503

Percentage Composition: C 79.97%; H 6.71%; O 13.32%

Melting Point: Mp 34°

Boiling Point: Bp_{0.5} 125-127°