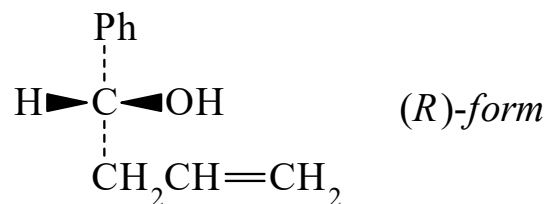




>>Entry Name: 1-Phenyl-3-buten-1-ol

Synonym(s): α -2-Propenylbenzenemethanol, 9CI. Allylphenylcarbinol



CAS Registry Number: 936-58-3

Molecular Formula: C₁₀H₁₂O

Molecular Weight: 148.204

Accurate Mass: 148.088815

Percentage Composition: C 81.04%; H 8.16%; O 10.80%

>>Variant: (R)-form

CAS Registry Number: 85551-57-1

Molecular Formula: C₁₀H₁₂O

Molecular Weight: 148.204

Accurate Mass: 148.088815

Percentage Composition: C 81.04%; H 8.16%; O 10.80%

Optical Rotation: $[\alpha]_{\text{D}}^{18} +48.3$ (C₆H₆)

>>Derivative: Hydrogen 3-nitrophthalate

Physical Description: Plates (C₆H₆/petrol)

Melting Point: Mp 126-127°

Optical Rotation: $[\alpha]_{\text{D}}^{18} +17.9$ (CHCl₃)

>>Derivative: Me ether

Synonym(s): 4-Methoxy-4-phenyl-1-butene

CAS Registry Number: 86766-46-3

Molecular Formula: C₁₁H₁₄O

Molecular Weight: 162.231

Accurate Mass: 162.104465

Percentage Composition: C 81.44%; H 8.70%; O 9.86%

Boiling Point: Bp_{0.1} 35-40°

Optical Rotation: $[\alpha]_{\text{D}}^{22} +35.02$ (c, 2.17 in CDCl₃)

>>Variant: (S)-form

CAS Registry Number: 77118-87-7

Molecular Formula: C₁₀H₁₂O

Molecular Weight: 148.204

Accurate Mass: 148.088815

Percentage Composition: C 81.04%; H 8.16%; O 10.80%

Boiling Point: Bp₁₅ 105-110°

Optical Rotation: $[\alpha]_{\text{D}}^{23} -44.92$ (c, 7.38 in C₆H₆) (96% ee)

>>Variant: (±)-form

CAS Registry Number: 80735-94-0

Molecular Formula: C₁₀H₁₂O

Molecular Weight: 148.204

Accurate Mass: 148.088815

Percentage Composition: C 81.04%; H 8.16%; O 10.80%

Boiling Point: Bp 228-229°. Bp₃ 88-90°

Density: d¹⁸ 1.004

Refractive Index: n_D^{21.5} 1.5289