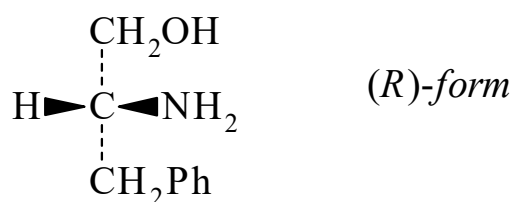




>>Entry Name: 2-Amino-3-phenyl-1-propanol

Synonym(s): β -Aminobenzenepropanol, 9CI. Phenylalaninol



Related CAS Registry Numbers(s): 104654-48-0 161972-38-9

Molecular Formula: C₉H₁₃NO

Molecular Weight: 151.208

Accurate Mass: 151.099714

Percentage Composition: C 71.49%; H 8.67%; N 9.26%; O 10.58%

Hazard & Toxicity: Dangerously exothermic syntheses reported

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 5267-64-1

Molecular Formula: C₉H₁₃NO

Molecular Weight: 151.208

Accurate Mass: 151.099714

Percentage Composition: C 71.49%; H 8.67%; N 9.26%; O 10.58%

Melting Point: Mp 96°

Optical Rotation: $[\alpha]_D^{21} +22.9$ (c, 3.36 in MeOH)

Aldrich: 28449-1

Fluka: 78115

Sigma: P9410

>>Derivative: *N*-tert-Butyloxycarbonyl

CAS Registry Number: 106454-69-7

Molecular Formula: C₁₄H₂₁NO₃

Molecular Weight: 251.325

Accurate Mass: 251.152144

Percentage Composition: C 66.91%; H 8.42%; N 5.57%; O 19.10%

Use/Importance: Chiral synthon

Physical Description: Cryst.

Melting Point: Mp 94-95°

Optical Rotation: $[\alpha]_D^{22} +22.1$ (c, 0.425 in CHCl₃)

Fluka: 15486

>>Derivative: *N*-Benzyloxycarbonyl

CAS Registry Number: 58917-85-4

Molecular Formula: C₁₇H₁₉NO₃

Molecular Weight: 285.342

Accurate Mass: 285.136494

Percentage Composition: C 71.56%; H 6.71%; N 4.91%; O 16.82%

Use/Importance: Chiral synthon

Physical Description: Cryst.

Melting Point: Mp 92-95°

Optical Rotation: $[\alpha]_D^{20} +43$ (c, 2 in MeOH)

Aldrich: 45993-3

Fluka: 97025

>>Derivative: Me ether

Synonym(s): 1-Methoxy-3-phenyl-2-propylamine. α -(Methoxymethyl)benzeneethanamine, 9CI

CAS Registry Number: 59919-07-2

Molecular Formula: C₁₀H₁₅NO

Molecular Weight: 165.235

Accurate Mass: 165.115364

Percentage Composition: C 72.69%; H 9.15%; N 8.48%; O 9.68%

Use/Importance: Enantioselective alkylating agent

Optical Rotation: $[\alpha]_D +14.3$ (c, 5.7 in C₆H₆)