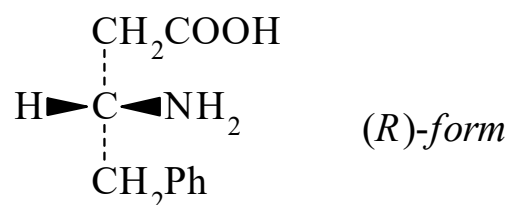




>>Entry Name: 3-Amino-4-phenylbutanoic acid, 8Cl

Synonym(s): β -Aminobenzenebutanoic acid, 9Cl. β -Homophenylalanine



Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

>>Variant: (*R*)-form

CAS Registry Number: 131270-08-1

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Optical Rotation: [α]_D²³ -8.5 (c, 0.2 in H₂O)

>>Derivative: Me ester

Molecular Formula: C₁₁H₁₅NO₂

Molecular Weight: 193.245

Accurate Mass: 193.110279

Percentage Composition: C 68.37%; H 7.82%; N 7.25%; O 16.56%

Physical Description: Cryst. (as hydrochloride)

Melting Point: Mp 133-134° (hydrochloride)

Optical Rotation: [α]_D²⁵ -9.2 (c, 1.5 in MeOH) (hydrochloride)

>>Variant: (*S*)-form

CAS Registry Number: 26250-87-3

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 231-232° (225-226°)

Optical Rotation: [α]_D +22.1 (c, 1.5 in H₂O)

>>Derivative: *N*-9-Fluorenylmethoxycarbonyl

CAS Registry Number: 193954-28-8

Molecular Formula: C₂₅H₂₃NO₄

Molecular Weight: 401.461

Accurate Mass: 401.162709

Percentage Composition: C 74.80%; H 5.77%; N 3.49%; O 15.94%

Physical Description: Cryst. (CHCl₃/hexane)

Optical Rotation: [α]_D -19.3 (c, 1.23 in CHCl₃)

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

CAS Registry Number: 131725-48-9

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 226°

References: