



>>Entry Name: Benzyloxycarbonylphenylalanine

Synonym(s): *N*-[(Phenylmethoxy)carbonyl]phenylalanine, 9Cl. *N*-Carboxy-3-phenylalanine *N*-benzyl ester, 8Cl. Z-PheOH

CAS Registry Number: 3588-57-6

PhCH₂OOCHNHCH(COOH)CH₂Ph

Molecular Formula: C₁₇H₁₇NO₄

Molecular Weight: 299.326

Accurate Mass: 299.115759

Percentage Composition: C 68.22%; H 5.72%; N 4.68%; O 21.38%

Sigma: C4252

>>Variant: D-form

CAS Registry Number: 2448-45-5

Molecular Formula: C₁₇H₁₇NO₄

Molecular Weight: 299.326

Accurate Mass: 299.115759

Percentage Composition: C 68.22%; H 5.72%; N 4.68%; O 21.38%

Melting Point: Mp 86-87°. Mp 100-101°

Optical Rotation: [α]_D -8.3 (EtOH). [α]_D²⁵ -1.6 (c, 2.0 in EtOH)

>>Derivative: Me ester

CAS Registry Number: 37440-07-6

Molecular Formula: C₁₈H₁₉NO₄

Molecular Weight: 313.352

Accurate Mass: 313.131409

Percentage Composition: C 69.00%; H 6.11%; N 4.47%; O 20.42%

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 80°

Optical Rotation: [α]_D²⁴ +1.6 (c, 2.5 in MeOH)

>>Derivative: 4-Nitrophenyl ester

CAS Registry Number: 2578-85-0

Molecular Formula: C₂₃H₂₀N₂O₆

Molecular Weight: 420.421

Accurate Mass: 420.132138

Percentage Composition: C 65.71%; H 4.79%; N 6.66%; O 22.83%

Physical Description: Cryst. (EtOAc/Et₂O)

Melting Point: Mp 121.5-123.5° (119-121°)

Optical Rotation: [α]_D²³ +23.9 (c, 2 in DMF)

>>Derivative: Pentachlorophenyl ester

CAS Registry Number: 81242-28-6

Molecular Formula: C₂₃H₁₆Cl₅NO₄

Molecular Weight: 547.647

Accurate Mass: 544.952194

Percentage Composition: C 50.44%; H 2.94%; Cl 32.37%; N 2.56%; O 11.69%

Physical Description: Cryst. (CH₂Cl₂/Et₂O/petrol)

Melting Point: Mp 150°

Optical Rotation: [α]_D²⁰ +53.9 (c, 1.02 in DMF)