



>>Entry Name: *N*-Glycylphenylalanine

Related CAS Registry Numbers(s): 62697-32-9

H2NCH2CONHCH(COOH)CH2Ph

Molecular Formula: C₁₁H₁₄N₂O₃

Molecular Weight: 222.243

Accurate Mass: 222.100443

Percentage Composition: C 59.45%; H 6.35%; N 12.60%; O 21.60%

>>Variant: D-form

CAS Registry Number: 34258-14-5

Molecular Formula: C₁₁H₁₄N₂O₃

Molecular Weight: 222.243

Accurate Mass: 222.100443

Percentage Composition: C 59.45%; H 6.35%; N 12.60%; O 21.60%

Optical Rotation: [α]_D²¹ -41.7 (c, 2.0 in H₂O)

Other: PB G04400

>>Variant: L-form

CAS Registry Number: 3321-03-7

Molecular Formula: C₁₁H₁₄N₂O₃

Molecular Weight: 222.243

Accurate Mass: 222.100443

Percentage Composition: C 59.45%; H 6.35%; N 12.60%; O 21.60%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 264-268°

Optical Rotation: [α]_D²⁵ +41.8 (c, 2.5 in H₂O)

Fluka: 50370

Sigma: G2752

>>Derivative: *N*-Benzyloxycarbonyl

CAS Registry Number: 1170-76-9

Molecular Formula: C₁₉H₂₀N₂O₅

Molecular Weight: 356.377

Accurate Mass: 356.137223

Percentage Composition: C 64.04%; H 5.66%; N 7.86%; O 22.45%

Melting Point: Mp 126.5-127.5°

Optical Rotation: [α]_D²⁵ +40.7 (c, 2.9 in EtOH)

Sigma: C0252

>>Derivative: *N*-Benzyloxycarbonyl, *tert*-butyl ester

CAS Registry Number: 16881-36-0

Molecular Formula: C₂₃H₂₈N₂O₅

Molecular Weight: 412.485

Accurate Mass: 412.199823

Percentage Composition: C 66.97%; H 6.84%; N 6.79%; O 19.39%

Physical Description: Cryst. (butanone/heptane)

Melting Point: Mp 62-63°

Optical Rotation: [α]_D²⁵ +10.2 (c, 2 in EtOH)

>>Derivative: *N*-Benzyloxycarbonyl, hydrazide

Molecular Formula: C₁₉H₂₂N₄O₄

Molecular Weight: 370.407

Accurate Mass: 370.164106

Percentage Composition: C 61.61%; H 5.99%; N 15.13%; O 17.28%

Physical Description: Needles (EtOH), or leaflets (EtOH/Et₂O)

Melting Point: Mp 104-105° (needles). Mp 164-165° (leaflets)

Optical Rotation: [α]_D²⁵ +5.1 (c, 2 in 0.5*M* HCl)