



>>Entry Name: *N*-Phenylalanylalanine, 9CI



Molecular Formula: C₁₂H₁₆N₂O₃

Molecular Weight: 236.27

Accurate Mass: 236.116093

Percentage Composition: C 61.00%; H 6.83%; N 11.86%; O 20.31%

>>Variant: L-L-form

CAS Registry Number: 3918-87-4

Molecular Formula: C₁₂H₁₆N₂O₃

Molecular Weight: 236.27

Accurate Mass: 236.116093

Percentage Composition: C 61.00%; H 6.83%; N 11.86%; O 20.31%

Optical Rotation: $[\alpha]_{\text{D}}^{25} +13.2$ (c, 2.1 in H₂O)

Sigma: P3251

>>Derivative: *N*-tert-Butyloxycarbonyl, Me ester

Molecular Formula: C₁₈H₂₆N₂O₅

Molecular Weight: 350.414

Accurate Mass: 350.184173

Percentage Composition: C 61.70%; H 7.48%; N 7.99%; O 22.83%

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 105°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -9$ (c, 1 in DMF)

>>Derivative: *N*-Benzyloxycarbonyl

Molecular Formula: C₂₀H₂₂N₂O₅

Molecular Weight: 370.404

Accurate Mass: 370.152873

Percentage Composition: C 64.85%; H 5.99%; N 7.56%; O 21.60%

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 165°

Optical Rotation: $[\alpha]_{\text{D}}^{22} -11$ (c, 2 in EtOH)

>>Derivative: *N*-Benzyloxycarbonyl, Me ester

Molecular Formula: C₂₁H₂₄N₂O₅

Molecular Weight: 384.431

Accurate Mass: 384.168523

Percentage Composition: C 65.61%; H 6.29%; N 7.29%; O 20.81%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 130-131°

>>Derivative: *N*-Benzyloxycarbonyl, amide

CAS Registry Number: 65118-54-9

Molecular Formula: C₂₀H₂₃N₃O₄

Molecular Weight: 369.419

Accurate Mass: 369.168857

Percentage Composition: C 65.03%; H 6.28%; N 11.37%; O 17.32%

Optical Rotation: $[\alpha]_{\text{D}}^{29} -8.86$ (c, 0.57 in MeOH)

References:

Grassmann, W. *et al.*, *Chem. Ber.*, 1958, **91**, 455, (*synth*)

Goldschmidt, S. *et al.*, *Chem. Ber.*, 1965, **98**, 2831, (*synth*)

Aboderin, A.A. *et al.*, *J.A.C.S.*, 1965, **87**, 5469, (*synth*)

Weitzel, G. *et al.*, *Hoppe Seyler's Z. Physiol. Chem.*, 1976, **357**, 187, (*synth*)

Puliti, R. *et al.*, *Acta Cryst. C*, 1996, **52**, 1820, (*cryst struct, amide, N-Ac*)

Khumtaveeporn, K. *et al.*, *Tetrahedron: Asymmetry*, 1999, **10**, 2563-2572, (*N-benzyloxycarbonyl amide*)