



>>Entry Name: *N*-Alanylphenylalanine

Extra CAS Registry Numbers(s): 1999-45-7

$\text{H}_3\text{CCH}(\text{NH}_2)\text{CONHCH}(\text{COOH})\text{CH}_2\text{Ph}$

Molecular Formula: $\text{C}_{12}\text{H}_{16}\text{N}_2\text{O}_3$

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: 3061-90-3

Molecular Formula: $\text{C}_{12}\text{H}_{16}\text{N}_2\text{O}_3$

Molecular Weight: 236.27

Accurate Mass: 236.116093

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

Optical Rotation: $[\alpha]_{\text{D}}^{25} +17$ (c, 1 in 1N HCl)

Sigma: A3128

>>Derivative: *N*-tert-Butyloxycarbonyl, hydrazide

CAS Registry Number: 2481-20-1

Molecular Formula: $\text{C}_{17}\text{H}_{26}\text{N}_4\text{O}_4$

Molecular Weight: 350.417

Accurate Mass: 350.195406

Percentage Composition: C 58.27%; H 7.48%; N 15.99%; O 18.26%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 162-163°

Optical Rotation: $[\alpha]_{\text{D}}^{22} -22.6$ (c, 1 in AcOH)

>>Derivative: *N*-Benzyloxycarbonyl

CAS Registry Number: 2768-53-8

Molecular Formula: $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_5$

Molecular Weight: 370.404

Accurate Mass: 370.152873

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

Physical Description: Prisms (MeOH aq.)

Melting Point: Mp 124-126°

Optical Rotation: $[\alpha]_{\text{D}}^{21} +39.2$ (c, 0.5 in dioxan)

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

CAS Registry Number: 3235-14-1

Molecular Formula: $\text{C}_{21}\text{H}_{24}\text{N}_2\text{O}_5$

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. (EtOAc/petrol)

Melting Point: Mp 99-100°

Optical Rotation: $[\alpha]_{\text{D}}^{22} -9.3$ (c, 1 in EtOH)

References:

Lübke, K. *et al.*, *Annalen*, 1964, **679**, 195, (*synth*)

Schröder, E., *Annalen*, 1964, **679**, 207, (*synth*)

Hirschmann, R. *et al.*, *J.O.C.*, 1967, **32**, 3415; 1971, **36**, 49, (*synth*)

Nagao, Y. *et al.*, *J.C.S. Perkin I*, 1984, 2439-2446, (*N*-benzyloxycarbonyl)