



>>Entry Name: Alanylalanylanine

$\text{H}_2\text{NCH}(\text{CH}_3)\text{CONHCH}(\text{CH}_3)\text{CONHCH}(\text{CH}_3)\text{COOH}$

Molecular Formula: $\text{C}_9\text{H}_{17}\text{N}_3\text{O}_4$

Molecular Weight: 231.251

Accurate Mass: 231.121907

Percentage Composition: C 46.75%; H 7.41%; N 18.17%; O 27.67%

>>Variant: (all-L)-form

CAS Registry Number: 5874-90-8

Molecular Formula: $\text{C}_9\text{H}_{17}\text{N}_3\text{O}_4$

Molecular Weight: 231.251

Accurate Mass: 231.121907

Percentage Composition: C 46.75%; H 7.41%; N 18.17%; O 27.67%

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

CAS Registry Number: 26910-17-8

Molecular Formula: $\text{C}_{12}\text{H}_{21}\text{N}_3\text{O}_5$

Molecular Weight: 287.315

Accurate Mass: 287.148122

Percentage Composition: C 50.17%; H 7.37%; N 14.63%; O 27.84%

Use/Importance: Substrate for elastase

Melting Point: Mp 254-255°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -147.5$ (c, 1.0 in H_2O)

Sigma: A5635

>>Derivative: *N*-Ac, Et ester

CAS Registry Number: 5686-38-4

Molecular Formula: $\text{C}_{13}\text{H}_{23}\text{N}_3\text{O}_5$

Molecular Weight: 301.342

Accurate Mass: 301.163772

Percentage Composition: C 51.82%; H 7.69%; N 13.94%; O 26.55%

Physical Description: Cryst. (trifluoroethanol/hexane)

Melting Point: Mp 246-247°

>>Derivative: *N*-Ac, 4-nitroanilide

CAS Registry Number: 40817-33-2

Molecular Formula: $\text{C}_{17}\text{H}_{23}\text{N}_5\text{O}_6$

Molecular Weight: 393.399

Accurate Mass: 393.164835

Percentage Composition: C 51.90%; H 5.89%; N 17.80%; O 24.40%

Use/Importance: Specific substrate for elastase

>>Derivative: *N*-Succinyl, 4-nitroanilide

CAS Registry Number: 52299-14-6

Molecular Formula: $\text{C}_{19}\text{H}_{25}\text{N}_5\text{O}_8$

Molecular Weight: 451.435

Accurate Mass: 451.170315

Percentage Composition: C 50.55%; H 5.58%; N 15.51%; O 28.35%

Use/Importance: Substrate for elastase

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 235-242°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +25$ (c, 0.7 in MeOH)

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 779C, (*ir*)

Goodman, M. *et al.*, *Biopolymers*, 1966, **4**, 275, (*synth*)

Gertler, A. *et al.*, *Can. J. Biochem.*, 1970, **48**, 384, (*synth*)

Feinstein, G. *et al.*, *Biochem. Biophys. Res. Commun.*, 1973, **50**, 1020, (*synth, use*)

Thomson, A. *et al.*, *Eur. J. Biochem.*, 1973, **38**, 1, (*synth, use*)

Okada, Y. *et al.*, *Chem. Pharm. Bull.*, 1985, **33**, 5301-5309, (*succinyl nitroanilide*)