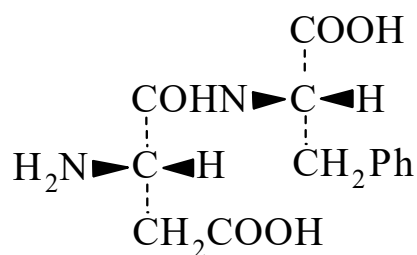




>>Entry Name: N^{α} -Aspartylphenylalanine
ENTRY UNDER REVIEW



Molecular Formula: $C_{13}H_{16}N_2O_5$
Molecular Weight: 280.28
Accurate Mass: 280.105923
Percentage Composition: C 55.71%; H 5.75%; N 9.99%; O 28.54%

>>Variant: L-L-form

CAS Registry Number: 13433-09-5

Molecular Formula: $C_{13}H_{16}N_2O_5$
Molecular Weight: 280.28
Accurate Mass: 280.105923
Percentage Composition: C 55.71%; H 5.75%; N 9.99%; O 28.54%
Source/Synthesis: Degradn. product of aspartame
Melting Point: Mp 232-235°
Optical Rotation: $[\alpha]_D +16$ (c, 1 in DMF)
Aldrich: 42166-9
Sigma: A7660

>>Derivative: Me ester
see Aspartame, [BDS15-X](#)

>>Derivative: *N*-(3,3-Dimethylbutyl), Me ester
Synonym(s): *N*-[*N*-(3,3-Dimethylbutyl)-L- α -aspartyl]-L-phenylalanine 1-methyl ester, 9Cl. Neotame

CAS Registry Number: 165450-17-9
Molecular Formula: $C_{20}H_{30}N_2O_5$
Molecular Weight: 378.467
Accurate Mass: 378.215473
Percentage Composition: C 63.47%; H 7.99%; N 7.40%; O 21.14%
Physical Description: Cryst. $+1H_2O$ (EtOAc/hexane)
Development Status: Submitted to FDA (1999) for approval as food sweetener
Melting Point: Mp 80-83° (monohydrate)
Optical Rotation: $[\alpha]_D -54.84$ (c, 1 in MeOH)
Other Data: Other diastereomers do not exhibit sweetening power

References:

Davey, J.M. *et al.*, *J.C.S.(C)*, 1966, 555, (*deriv*)
Mazur, R.H. *et al.*, *J.A.C.S.*, 1969, **91**, 2684, (*synth*)
Roberts, G.C.K. *et al.*, *Biochem. J.*, 1971, **125**, 88P, (*pmr*)
Yasutake, A. *et al.*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 2413, (*deriv*)
U.S. Pat., 1996, 5 510 508; *CA*, **124**, 203104p, (*Neotame*)
Hutchinson, S.A. *et al.*, *Food Rev. Int.*, 1999, **15**, 249-261, (*formn*)
Prakash, I. *et al.*, *Synth. Commun.*, 1999, **29**, 4461-4467, (*synth, cryst struct, pmr, Neotame*)