



>>Entry Name: N^{β} -Aspartylglutamic acid

Related CAS Registry Numbers(s): 57096-36-3
HOOCCH(NH2)CH2CONHCH(COOH)CH2CH2COOH

Molecular Formula: $C_9H_{14}N_2O_7$

Molecular Weight: 262.219

Accurate Mass: 262.080103

Percentage Composition: C 41.22%; H 5.38%; N 10.68%; O 42.71%

>>Variant: L-L-form

CAS Registry Number: 68006-14-4

Molecular Formula: $C_9H_{14}N_2O_7$

Molecular Weight: 262.219

Accurate Mass: 262.080103

Percentage Composition: C 41.22%; H 5.38%; N 10.68%; O 42.71%

Other Data: Extremely hygroscopic

>>Derivative: *N*-Ac

Synonym(s): Spaglumatic acid, INN‡

CAS Registry Number: 4910-46-7

Molecular Formula: $C_{11}H_{16}N_2O_8$

Molecular Weight: 304.256

Accurate Mass: 304.090668

Percentage Composition: C 43.42%; H 5.30%; N 9.21%; O 42.07%

Use/Importance: Sedative, used as Ca salt

Melting Point: Mp 115-116 dec.°

Optical Rotation: $[\alpha]_D^{24} -37.5$ (c, 2 in H_2O)

Calculated Log P Data: Log P -2.19 (calc)

Sigma: A9436

References:

Le Quesne, W.J. *et al.*, *J.C.S.*, 1952, 24

Losse, G. *et al.*, *Chem. Ber.*, 1964, **97**, 1789

Marchetti, E. *et al.*, *Ann. Chim. (Rome)*, 1967, **57**, 624, (*synth, pharmacol*)

Ger. Pat., 1975, 2 500 802; *CA*, **83**, 179624v, (*synth, pharmacol*)