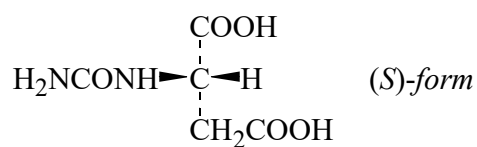




>>Entry Name: *N*-(Aminocarbonyl)aspartic acid

Synonym(s): *N*-Carbamoylaspartic acid. Ureidosuccinic acid



CAS Registry Number: 1116-06-9

Related CAS Registry Numbers(s): 16649-79-9 16649-80-2 16649-82-4 30905-63-6 74078-74-3

Molecular Formula: $\text{C}_5\text{H}_8\text{N}_2\text{O}_5$

Molecular Weight: 176.129

Accurate Mass: 176.043323

Percentage Composition: C 34.10%; H 4.58%; N 15.91%; O 45.42%

Source/Synthesis: Biosynthetic precursor of orotic acid in pyrimidine synth.

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 16649-81-3

Molecular Formula: $\text{C}_5\text{H}_8\text{N}_2\text{O}_5$

Molecular Weight: 176.129

Accurate Mass: 176.043323

Percentage Composition: C 34.10%; H 4.58%; N 15.91%; O 45.42%

Physical Description: Cryst.

Melting Point: Mp 128-130°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -18.6$ (c, 0.64 in H_2O)

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 13184-27-5

Molecular Formula: $\text{C}_5\text{H}_8\text{N}_2\text{O}_5$

Molecular Weight: 176.129

Accurate Mass: 176.043323

Percentage Composition: C 34.10%; H 4.58%; N 15.91%; O 45.42%

Physical Description: Hemispheric cryst. (Me_2CO)

Melting Point: Mp 128-130°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +18.9$ (c, 3.38 in H_2O)

>>Variant: ($\pm$)-form

CAS Registry Number: 923-37-5

Molecular Formula: $\text{C}_5\text{H}_8\text{N}_2\text{O}_5$

Molecular Weight: 176.129

Accurate Mass: 176.043323

Percentage Composition: C 34.10%; H 4.58%; N 15.91%; O 45.42%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 178-180°

References:

Nyc, J.F. *et al.*, *J.A.C.S.*, 1947, **69**, 1382-1384, (*synth*)

Reichard, P., *Adv. Enzymol.*, 1959, **21**, 263-294, (*biochem*)

Miyazaki, H. *et al.*, *Chem. Pharm. Bull.*, 1967, **15**, 1604-1606, (*enantiomers, synth*)

Bruce, M.J. *et al.*, *J.C.S. Perkin 2*, 1994, 319-321, (*synth, cmr*)