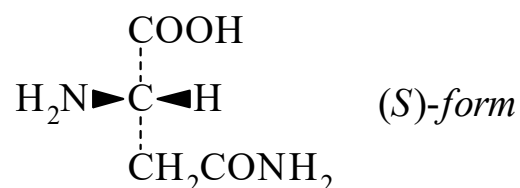




>>Entry Name: Asparagine, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2,4-Diamino-4-oxobutanoic acid. Aspartic acid β -monoamide. β -Asparagine. Asparamide. Altheine. Asn



CAS Registry Number: 7006-34-0

Related CAS Registry Numbers(s): 5794-13-8

Molecular Formula: $\text{C}_4\text{H}_8\text{N}_2\text{O}_3$

Molecular Weight: 132.119

Accurate Mass: 132.053493

Percentage Composition: C 36.36%; H 6.10%; N 21.20%; O 36.33%

General Statement: Derivs. labelled *N* (here and in 9CI) refer to those subst. on the amide (or N^4) nitrogen; N^2 refers to subst. on amino group

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 2058-58-4

Extra CAS Registry Numbers(s): 5794-24-1

Molecular Formula: $\text{C}_4\text{H}_8\text{N}_2\text{O}_3$

Molecular Weight: 132.119

Accurate Mass: 132.053493

Percentage Composition: C 36.36%; H 6.10%; N 21.20%; O 36.33%

Physical Description: Cryst. + H_2O

Melting Point: Mp 234-235°

Optical Rotation: $[\alpha]_{\text{D}}^{15} +5.4$ (H_2O)

Aldrich: 44159-7

Fluka: 11155

>>Derivative: *N*-Hydroxy

CAS Registry Number: 36244-81-2

Molecular Formula: $\text{C}_4\text{H}_8\text{N}_2\text{O}_4$

Molecular Weight: 148.118

Accurate Mass: 148.048408

Percentage Composition: C 32.44%; H 5.44%; N 18.91%; O 43.21%

Physical Description: Cryst. (EtOH aq.)

Optical Rotation: $[\alpha]_{\text{D}}^{25} -27.7$ (c, 2 in HCl aq.)

Sigma: A9009

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 70-47-3

Molecular Formula: $\text{C}_4\text{H}_8\text{N}_2\text{O}_3$

Molecular Weight: 132.119

Accurate Mass: 132.053493

Percentage Composition: C 36.36%; H 6.10%; N 21.20%; O 36.33%

Biological Source: Widely distributed in the plant kingdom. Isol. from asparagus, beetroot, peas, beans, etc.

Use/Importance: One of the nonessential amino acids. Dietary supplement, nutrient

Physical Description: Rhombic hemihedral cryst. + H_2O (H_2O)

Melting Point: Mp 234-235° (rapid heat). Mp 226-227 dec.° (slow heat)

Optical Rotation: $[\alpha]_{\text{D}}^{25} -7.4$ (c, 2 in H_2O). $[\alpha]_{\text{D}} +33.2$ (3*M* HCl)

Solubility: Mod. sol. H_2O (3.1g/100g at 25°)

pKa Value: $\text{p}K_{\text{a}2}$ 8.6 (NH_2)

Other Data: Isoelectric point 5.41. Bitter taste

Aldrich: A9300-3

Fluka: 11149

Sigma: A0884