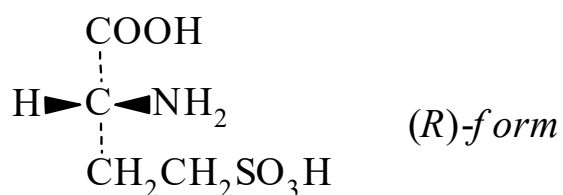




>>Entry Name: 2-Amino-4-sulfobutanoic acid, 9CI

Synonym(s): Homocysteic acid



CAS Registry Number: 1001-13-4

Molecular Formula: C₄H₉NO₅S

Molecular Weight: 183.185

Accurate Mass: 183.020144

Percentage Composition: C 26.23%; H 4.95%; N 7.65%; O 43.67%; S 17.50%

Hazard & Toxicity: Neurotoxin

>>Variant: (*R*)-form

CAS Registry Number: 56892-03-6

Molecular Formula: C₄H₉NO₅S

Molecular Weight: 183.185

Accurate Mass: 183.020144

Percentage Composition: C 26.23%; H 4.95%; N 7.65%; O 43.67%; S 17.50%

Biological Source: Isol. from the red alga *Palmaria palmata*

Physical Description: Cryst. (H₂O/EtOH/Et₂O)

Melting Point: Mp 270 dec.°. Mp 267°

Optical Rotation: [α]_D²⁵−10 (c, 5 in 1M HCl). [α]_D²¹−18 (c, 1.305 in H₂O)

Other Data: Isol. partially racemised

Sigma: H9883

>>Variant: (*S*)-form

CAS Registry Number: 14857-77-3

Molecular Formula: C₄H₉NO₅S

Molecular Weight: 183.185

Accurate Mass: 183.020144

Percentage Composition: C 26.23%; H 4.95%; N 7.65%; O 43.67%; S 17.50%

Physical Description: Cryst. (H₂O/EtOH/Et₂O)

Melting Point: Mp 261°

Optical Rotation: [α]_D¹⁹+17 (c, 0.57 in H₂O)

>>Derivative: *N*-Benzyloxycarbonyl, *S*-amide

CAS Registry Number: 112898-30-3

Molecular Formula: C₁₂H₁₆N₂O₆S

Molecular Weight: 316.334

Accurate Mass: 316.072908

Percentage Composition: C 45.56%; H 5.10%; N 8.86%; O 30.35%; S 10.14%

Melting Point: Mp 78-82°

Optical Rotation: [α]_D²¹−10 (c, 1 in H₂O)

Other Data: Comly. available; props. given are from catalogue data

>>Variant: (±)-form

CAS Registry Number: 504-33-6

Molecular Formula: C₄H₉NO₅S

Molecular Weight: 183.185

Accurate Mass: 183.020144

Percentage Composition: C 26.23%; H 4.95%; N 7.65%; O 43.67%; S 17.50%

Physical Description: Cryst. (H₂O)

Aldrich: 21974-6

Sigma: H2257

References: