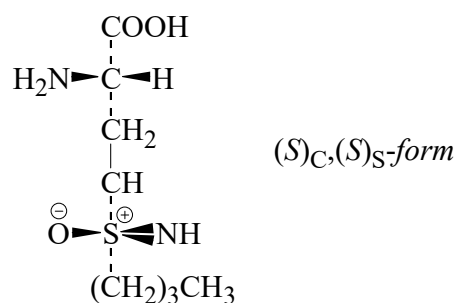




>>Entry Name: 2-Amino-4-(S-butylsulfonimidoyl)butanoic acid, 9CI

Synonym(s): S-(3-Amino-3-carboxypropyl)-S-butylsulfoximine. Buthionine sulfoximine. BSO. NSC 326231



CAS Registry Number: 5072-26-4

Related CAS Registry Numbers(s): 71765-30-5 83730-53-4 97590-40-4 113158-69-3 113158-70-6 148968-82-5

Molecular Formula: $C_8H_{18}N_2O_3S$

Molecular Weight: 222.308

Accurate Mass: 222.103813

Percentage Composition: C 43.22%; H 8.16%; N 12.60%; O 21.59%; S 14.42%

Biological Use/Importance: Glutathione biosynth. inhibitor. Radiosensitiser used in cancer chemotherapy. Pharmacol. tool for decreasing cellular GSH levels

Other Data: Preparations used as drugs may consist of diastereoisomeric mixtures

>>Variant: $(S)_C, (S)_S\text{-form}$

CAS Registry Number: 113158-67-1

Molecular Formula: $C_8H_{18}N_2O_3S$

Molecular Weight: 222.308

Accurate Mass: 222.103813

Percentage Composition: C 43.22%; H 8.16%; N 12.60%; O 21.59%; S 14.42%

Optical Rotation: $[\alpha]_D^{20} +34$ (c, 2.0 in 1M HCl)

Other Data: Pharmacol. active isomer

>>Variant: $(S)_C, (R)_S\text{-form}$

CAS Registry Number: 113158-68-2

Molecular Formula: $C_8H_{18}N_2O_3S$

Molecular Weight: 222.308

Accurate Mass: 222.103813

Percentage Composition: C 43.22%; H 8.16%; N 12.60%; O 21.59%; S 14.42%

Optical Rotation: $[\alpha]_D^{20} +33.7$ (c, 2.0 in 1M HCl)

>>Variant: $(S)_C, (\pm)_S\text{-form}$

Synonym(s): L-form

CAS Registry Number: 83730-53-4

Molecular Formula: $C_8H_{18}N_2O_3S$

Molecular Weight: 222.308

Accurate Mass: 222.103813

Percentage Composition: C 43.22%; H 8.16%; N 12.60%; O 21.59%; S 14.42%

Physical Description: Cryst.

Melting Point: Mp 224-226°

Optical Rotation: $[\alpha]_D^{20} +33$ (c 1.0, 1M HCl)

Other Data: Mixt. of diastereomers at S atom

>>Variant: $(\pm)\text{-form}$

CAS Registry Number: 97590-40-4

Molecular Formula: $C_8H_{18}N_2O_3S$

Molecular Weight: 222.308

Accurate Mass: 222.103813

Percentage Composition: C 43.22%; H 8.16%; N 12.60%; O 21.59%; S 14.42%

Physical Description: Needles (EtOH)

Melting Point: Mp 214°

References: