



>>Derivative: S-Benzyl

Molecular Formula: C₁₁H₁₅NO₂S

Molecular Weight: 225.311

Accurate Mass: 225.082349

Percentage Composition: C 58.64%; H 6.71%; N 6.22%; O 14.20%; S 14.23%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 210-211° (244-246° dec.)

Optical Rotation: [α]_D²⁶+27.2 (c, 2 in 2M HCl)

>>Variant: (±)-form

CAS Registry Number: 454-29-5

Molecular Formula: C₄H₉NO₂S

Molecular Weight: 135.187

Accurate Mass: 135.035399

Percentage Composition: C 35.54%; H 6.71%; N 10.36%; O 23.67%; S 23.72%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 232-233° (263-265° dec.)

pKa Value: pK_{a2} 8.87; pK_{a3} 10.86 (25°)

Aldrich: 19314-3

Fluka: 53510

Sigma: H4628

>>Derivative: Thiolactone

see 3-Aminodihydro-2(3*H*)-thiophenone, [LTV38-J](#)

>>Derivative: S-Et

see Ethionine, [CJC20-U](#)

>>Derivative: S-Propyl

Molecular Formula: C₁₀H₁₅NO₂S

Molecular Weight: 213.3

Accurate Mass: 213.082349

Percentage Composition: C 56.31%; H 7.09%; N 6.57%; O 15.00%; S 15.03%

Melting Point: Mp 250-252 dec.°

>>Derivative: S-Butyl

Synonym(s): Buthionine

CAS Registry Number: 3343-64-4

Molecular Formula: C₈H₁₇NO₂S

Molecular Weight: 191.294

Accurate Mass: 191.097999

Percentage Composition: C 50.23%; H 8.96%; N 7.32%; O 16.73%; S 16.76%

Melting Point: Mp 238-243°

Sigma: B8638

>>Derivative: S-Benzyl

Molecular Formula: C₁₁H₁₅NO₂S

Molecular Weight: 225.311

Accurate Mass: 225.082349

Percentage Composition: C 58.64%; H 6.71%; N 6.22%; O 14.20%; S 14.23%

Melting Point: Mp 240-250°

References: