



>>Entry Name: Bis(2-aminoethyl) disulfide

ENTRY UNDER REVIEW

Synonym(s): 2,2'-Dithiobisethanamine, 9Cl. 2,2'-Dithiobisethylamine, 8Cl. Cystamine. Cystineamine. L 1591

CAS Registry Number: 51-85-4

Related CAS Registry Numbers(s): 16214-16-7

$\text{H}_2\text{NCH}_2\text{CH}_2\text{SSCH}_2\text{CH}_2\text{NH}_2$

Molecular Formula: $\text{C}_4\text{H}_{12}\text{N}_2\text{S}_2$

Molecular Weight: 152.284

Accurate Mass: 152.044188

Percentage Composition: C 31.55%; H 7.94%; N 18.40%; S 42.11%

Use/Importance: Radioprotective agent

Physical Description: Viscous oil

Calculated Log P Data: Log P -0.23 (calc)

Other Data: Dec. on dist.

Hazard & Toxicity: LD₅₀ (mus, ipr) 220 mg/kg

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 56-17-7

Physical Description: Prisms (EtOH)

Melting Point: Mp 212°

Hazard & Toxicity: LD₅₀ (mus, ipr) 405 mg/kg. Exp. reprod. effects

Aldrich: C12150-9

Fluka: 30050

Sigma: C8707

>>Derivative: Dipicrate

Physical Description: Yellow cryst.

Melting Point: Mp 204°

>>Derivative: S-Oxide

Synonym(s): Cystamine monosulfoxide

Molecular Formula: $\text{C}_4\text{H}_{12}\text{N}_2\text{OS}_2$

Molecular Weight: 168.284

Accurate Mass: 168.039103

Percentage Composition: C 28.55%; H 7.19%; N 16.65%; O 9.51%; S 38.11%

Physical Description: Needles (EtOH aq.) (as ditosylate)

Melting Point: Mp 160 dec.° (ditosylate)

>>Derivative: S,S'-Dioxide

Synonym(s): 2,2'-Disulfinylbisethanamine, 9Cl. Cystamine disulfoxide

CAS Registry Number: 4747-26-6

Molecular Formula: $\text{C}_4\text{H}_{12}\text{N}_2\text{O}_2\text{S}_2$

Molecular Weight: 184.283

Accurate Mass: 184.034018

Percentage Composition: C 26.07%; H 6.56%; N 15.20%; O 17.36%; S 34.80%

Melting Point: Mp 166° (154-155° dec.) (as hydrochloride)

Other Data: May be a mixt. of diastereoisomers at S