



Sigma: D1019

>>Derivative: *N,N*-Di-Me

Synonym(s): 2-(Dimethylamino)ethanethiol, 9Cl, 8Cl. **Captamine**, INN

CAS Registry Number: 108-02-1

Molecular Formula: C₄H₁₁NS

Molecular Weight: 105.204

Accurate Mass: 105.061219

Percentage Composition: C 45.67%; H 10.54%; N 13.31%; S 30.48%

Use/Importance: Depigmentation agent

Physical Description: Liq.

Boiling Point: Bp 120-127°. Bp₄₀ 45-47°

pKa Value: pK_{a1} 10.9 (20°,25% EtOH)

Hazard & Toxicity: LD₅₀ (mus, scu) 214 mg/kg

>>Derivative: *N,N*-Di-Me; hydrochloride

Synonym(s): Captamine hydrochloride, USAN. NSC 45463

CAS Registry Number: 13242-44-9

Physical Description: Solid

Melting Point: Mp 156-157°

Aldrich: D14100-3

Fluka: 39010

>>Derivative: *N,N*-Di-Me, *S*-Ac

Synonym(s): *S*-[2-(Dimethylamino)ethyl] ethanethioate, 9Cl

CAS Registry Number: 18719-14-7

Molecular Formula: C₆H₁₃NOS

Molecular Weight: 147.241

Accurate Mass: 147.071784

Percentage Composition: C 48.94%; H 8.90%; N 9.51%; O 10.87%; S 21.78%

Melting Point: Mp 145° (as hydrochloride)

>>Derivative: *N,N*-Di-Et

CAS Registry Number: 1942-52-5

Extra CAS Registry Numbers(s): 100-38-9

Molecular Formula: C₆H₁₅NS

Molecular Weight: 133.257

Accurate Mass: 133.092519

Percentage Composition: C 54.08%; H 11.35%; N 10.51%; S 24.06%

Use/Importance: Used as 0.1% aq. soln. for simultaneous photometric detn. of Rh and Pd ($\lambda_{\max}$ 258, 303 nm)

Physical Description: Solid (as hydrochloride)

Solubility: Sol. H₂O, EtOH

pKa Value: pK_{a2} 11.01 (NEt₂)

Aldrich: D8660-4

Fluka: 31770

Sigma: D3753

>>Derivative: *N,N*-Diisopropyl

>>Derivative: *N*-Butyl

Synonym(s): 2-(Butylamino)ethanethiol, 9Cl, 8Cl

CAS Registry Number: 5842-00-2

Molecular Formula: C₆H₁₅NS

Molecular Weight: 133.257

Accurate Mass: 133.092519

Percentage Composition: C 54.08%; H 11.35%; N 10.51%; S 24.06%

Physical Description: Liq.

Boiling Point: Bp₂ 740°

Refractive Index: n