



>>Entry Name: 3-Amino-1-propanethiol, 9Cl

Synonym(s): 3-Aminopropyl mercaptan. 3-Mercaptopropylamine. Homocysteamine

CAS Registry Number: 462-47-5

Related CAS Registry Numbers(s): 13139-95-2 13448-87-8 29205-72-9

HSCH₂CH₂CH₂NH₂

Molecular Formula: C₃H₉NS

Molecular Weight: 91.177

Accurate Mass: 91.045569

Percentage Composition: C 39.52%; H 9.95%; N 15.36%; S 35.17%

Physical Description: Cryst.

Melting Point: Mp 112-113°

Hazard & Toxicity: LD₅₀ (mus, ipr) 125 mg/kg

>>Derivative: Hydrochloride

CAS Registry Number: 7211-54-3

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 69°

Hazard & Toxicity: LD₅₀ (mus, ipr) 175 mg/kg

>>Derivative: Disulfide

Synonym(s): 3,3'-Dithiobis-1-propanamine, 9Cl. 3,3'-Diaminodipropyl disulfide. Homocystamine

CAS Registry Number: 463-22-9

Molecular Formula: C₆H₁₆N₂S₂

Molecular Weight: 180.338

Accurate Mass: 180.075488

Percentage Composition: C 39.96%; H 8.94%; N 15.53%; S 35.56%

Physical Description: Solid (EtOH/Et₂O) (as hydrobromide)

>>Derivative: Disulfide, picrate

Melting Point: Mp 145-146°

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

Synonym(s): 3-Mercapto-*N,N,N*-trimethyl-1-propanaminium(1+), 9Cl. (3-Mercaptopropyl)trimethylammonium, 8Cl

CAS Registry Number: 14617-77-7

Molecular Formula: C₆H₁₆NS⁽⁺⁾

Molecular Weight: 134.265

Accurate Mass: 134.100344

Percentage Composition: C 53.67%; H 12.01%; N 10.43%; S 23.88%

Physical Description: Cryst. (EtOH) (as iodide)

Melting Point: Mp 187-188° (iodide)

References:

- Schöberl, A. *et al.*, *Annalen*, 1958, **66**, 66, (*disulfide*)
Turk, S.D. *et al.*, *J.O.C.*, 1962, **27**, 2846, (*synth*)
Suyama, T. *et al.*, *Yakugaku Zasshi*, 1964, **84**, 1012; *CA*, **62**, 6552f, (*synth, deriv*)
Ekambaram, A. *et al.*, *J.O.C.*, 1967, **32**, 2985, (*N-tri-Me*)
Hartmann, T., *Naturwissenschaften*, 1968, **55**, 391, (*isol, deriv*)
DeMarco, C. *et al.*, *Anal. Biochem.*, 1973, **51**, 265, (*synth*)
Dalgaard, L. *et al.*, *Phytochemistry*, 1977, **16**, 931, (*isol, deriv*)