



>>Entry Name: 3-(Methylthio)propylamine, 8Cl

Synonym(s): 3-(Methylthio)propanamine, 9Cl. 3-Methylmercaptopropylamine. 3-Aminopropyl methyl sulfide

CAS Registry Number: 4104-45-4

$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{SMe}$

Molecular Formula: $\text{C}_4\text{H}_{11}\text{NS}$

Molecular Weight: 105.204

Accurate Mass: 105.061219

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

Biological Source: Formed by *Streptomyces* from Methionine. Constit. of *Iberis amara* and from the brown alga *Desmarestia aculeata*

Physical Description: Steam-volatile liq.

Boiling Point: Bp 170°. Bp₁₄ 66-67°

Solubility: Misc. H_2O , EtOH, Et₂O

Other: PB M29080

>>Derivative: Hydrochloride

CAS Registry Number: 2419-62-7

Physical Description: Hygroscopic needles (Me_2CO)

Melting Point: Mp 144°

>>Derivative: Picrate

Physical Description: Cryst.

Melting Point: Mp 126-127°

>>Derivative: S-Oxide

Synonym(s): 3-(Methylsulfinyl)propylamine

Molecular Formula: $\text{C}_4\text{H}_{11}\text{NOS}$

Molecular Weight: 121.203

Accurate Mass: 121.056134

Percentage Composition: C 39.64%; H 9.15%; N 11.56%; O 13.20%; S 26.46%

Physical Description: Cryst.

Melting Point: Mp 27°

Boiling Point: Bp_{0.04} 90-91°

>>Derivative: S,S-Dioxide

Synonym(s): 3-(Methylsulfonyl)propylamine

Molecular Formula: $\text{C}_4\text{H}_{11}\text{NO}_2\text{S}$

Molecular Weight: 137.202

Accurate Mass: 137.051049

Percentage Composition: C 35.02%; H 8.08%; N 10.21%; O 23.32%; S 23.37%

Physical Description: Hygroscopic cryst.

Melting Point: Mp 44°

Boiling Point: Bp₆ 165-168°

References:

Schneider, W., *Annalen*, 1910, **375**, 207, (synth)

Karrer, P. *et al.*, *Helv. Chim. Acta*, 1950, **33**, 1237, (synth)

Dose, K., *Chem. Ber.*, 1957, **90**, 1251, (synth)

Suyama, T. *et al.*, *Yakugaku Zasshi*, 1964, **84**, 1012; *CA*, **62**, 6552, (synth)

Pesch, R. *et al.*, *Org. Mass Spectrom.*, 1974, **9**, 861, (ms)