



>>Entry Name: 3-Mercapto-1-propanol, 9CI
ENTRY UNDER REVIEW

CAS Registry Number: 19721-22-3

HOCH₂CH₂CH₂SH

Molecular Formula: C₃H₈OS

Molecular Weight: 92.162

Accurate Mass: 92.029585

Percentage Composition: C 39.10%; H 8.75%; O 17.36%; S 34.79%

Use/Importance: Derivatisation reagent in hplc. anal. of primary amines

Physical Description: Liq. with unpleasant odour

Boiling Point: Bp₁₄ 87°. Bp₉ 72-73°

Aldrich: 40573-6

Fluka: 63766

Rare Chemicals Library: S87989-4

>>Derivative: O-Ac

CAS Registry Number: 26473-61-0

Molecular Formula: C₅H₁₀O₂S

Molecular Weight: 134.199

Accurate Mass: 134.04015

Percentage Composition: C 44.75%; H 7.51%; O 23.84%; S 23.89%

Boiling Point: Bp₂₀ 87°. Bp_{1.5} 58°

Rare Chemicals Library: S78668-3

>>Derivative: S-Ac

Molecular Formula: C₅H₁₀O₂S

Molecular Weight: 134.199

Accurate Mass: 134.04015

Percentage Composition: C 44.75%; H 7.51%; O 23.84%; S 23.89%

Boiling Point: Bp₄ 92°. Bp_{0.3} 57°

>>Derivative: Di-Ac

Molecular Formula: C₇H₁₂O₃S

Molecular Weight: 176.236

Accurate Mass: 176.050715

Percentage Composition: C 47.71%; H 6.86%; O 27.24%; S 18.19%

Boiling Point: Bp₁₉ 120-121°

>>Derivative: S-Me

Synonym(s): 3-(Methylthio)-1-propanol. FEMA 3415. 3-Hydroxypropyl methyl sulfide

CAS Registry Number: 505-10-2

Molecular Formula: C₄H₁₀OS

Molecular Weight: 106.188

Accurate Mass: 106.045235

Percentage Composition: C 45.24%; H 9.49%; O 15.07%; S 30.20%

Biological Source: Aroma constit. of wines etc., fermentation prod. of *Saccharomyces cerevisiae*

Boiling Point: Bp₁₃ 89-90°. Bp₆ 72-72.5°

Density: d₄⁴ 1.03

Refractive Index: n_D²⁰ 1.4832

Aldrich: W34150-9

>>Derivative: S-Me, O-Ac

CAS Registry Number: 16630-55-0

Molecular Formula: C₆H₁₂O₂S

Molecular Weight: 148.226

Accurate Mass: 148.0558

Percentage Composition: C 48.62%; H 8.16%; O 21.59%; S 21.63%

Boiling Point: Bp₁₄ 96°