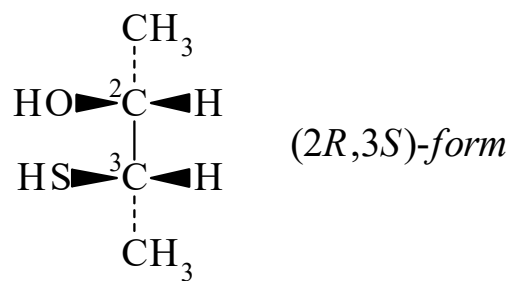




>>Entry Name: 3-Mercapto-2-butanol, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3502



CAS Registry Number: 54812-86-1

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%

Hazard & Toxicity: Odour induces nausea

Aldrich: 26479-2

>>Variant: (2*R*,3*S*)-form

Synonym(s): (+)-*erythro*-form

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%

Boiling Point: Bp₃₁ 73.5-74°

Optical Rotation: [α]_D²⁵+16

Refractive Index: n_D²⁵ 1.4783

Other Data: Hygroscopic

>>Variant: (2*RS*,3*RS*)-form

Synonym(s): (±)-*threo*-form

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%

Boiling Point: Bp₁₀ 53°

>>Derivative: *S*-Me

Synonym(s): 3-(Methylthio)-2-butanol

CAS Registry Number: 27022-36-2

Molecular Formula: C₅H₁₂OS

Molecular Weight: 120.215

Accurate Mass: 120.060885

Percentage Composition: C 49.96%; H 10.06%; O 13.31%; S 26.67%

Boiling Point: Bp₂₅ 78°

>>Derivative: Me ether

Synonym(s): 2-Mercapto-3-methoxybutane. 3-Methoxy-2-butanethiol

Molecular Formula: C₅H₁₂OS

Molecular Weight: 120.215

Accurate Mass: 120.060885

Percentage Composition: C 49.96%; H 10.06%; O 13.31%; S 26.67%

Boiling Point: Bp₁₀₀ 70°

>>Derivative: *O,S*-Di-Me

Synonym(s): 2-Methoxy-3-(methylthio)butane