



>>Entry Name: 3-Methyl-2-butene-1-thiol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Dimethylallyl mercaptan

CAS Registry Number: 5287-45-6

$(\text{H}_3\text{C})_2\text{C}=\text{CHCH}_2\text{SH}$

Molecular Formula: $\text{C}_5\text{H}_{10}\text{S}$

Molecular Weight: 102.2

Accurate Mass: 102.05032

Percentage Composition: C 58.76%; H 9.86%; S 31.38%

Biological Source: Substance responsible for ``sun-struck" flavour of beer

Physical Description: Liq. with leek-like aroma

Boiling Point: Bp 125.5-127°

>>Derivative: S-Ac

Synonym(s): S-(3-Methyl-2-butenyl) ethanethioate. S-Prenyl thioacetate

CAS Registry Number: 33049-93-3

Molecular Formula: $\text{C}_7\text{H}_{12}\text{OS}$

Molecular Weight: 144.237

Accurate Mass: 144.060885

Percentage Composition: C 58.29%; H 8.39%; O 11.09%; S 22.23%

Biological Source: Constit. of the essential oil of *Phyllosma capensis*

Boiling Point: Bp₂ 70-72°

>>Derivative: S-(2-Methylpropanoyl)

Synonym(s): S-(3-Methyl-2-butenyl) 2-methylpropanethioate. S-Prenyl thioisobutyrate

CAS Registry Number: 53626-94-1

Molecular Formula: $\text{C}_9\text{H}_{16}\text{OS}$

Molecular Weight: 172.291

Accurate Mass: 172.092185

Percentage Composition: C 62.74%; H 9.36%; O 9.29%; S 18.61%

Biological Source: Constit. of buchu (*Agathosma*) spp. and *Phyllosma capensis*

Boiling Point: Bp₁₅ 100°

UV: [neutral] λ_{max} 206 (ϵ 6800); 234 (ϵ 5300) (no solvent reported)

>>Derivative: S-(3-Methylbutanoyl)

Synonym(s): S-(3-Methyl-2-butenyl) 3-methylbutanethioate. S-Prenyl thioisovalerate

CAS Registry Number: 75631-91-3

Molecular Formula: $\text{C}_{10}\text{H}_{18}\text{OS}$

Molecular Weight: 186.318

Accurate Mass: 186.107835

Percentage Composition: C 64.47%; H 9.74%; O 8.59%; S 17.21%

Biological Source: Constit. of the essential oil of *Phyllosma capensis*

Boiling Point: Bp₄ 88-92°

References:

- Kuroiwa, Y. *et al.*, *Agric. Biol. Chem.*, 1961, **25**, 257, (*isol*)
Obota, Y. *et al.*, *Nature (London)*, 1961, **190**, 635, (*isol, synth*)
Moore, C.G. *et al.*, *Tetrahedron*, 1962, **18**, 205, (*synth*)
Rivett, D.E.A. *et al.*, *Tet. Lett.*, 1974, 1253, (*isol, ester*)
Lui, K.-C. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 1019, (*synth*)
Campbell, W.E. *et al.*, *Phytochemistry*, 1980, **19**, 1537, (*isol, esters*)