



>>Entry Name: Methyl (methylthio)methyl disulfide, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2,3,5-Trithiahexane

CAS Registry Number: 42474-44-2

MeSSCH₂SMe

Molecular Formula: C₃H₈S₃

Molecular Weight: 140.294

Accurate Mass: 139.97881

Percentage Composition: C 25.68%; H 5.75%; S 68.57%

Source/Synthesis: Found in essential oil of hops and in Camembert cheeses, cooked cabbage, broccoli and cauliflower

Physical Description: Sl. yellow liq.

Boiling Point: Bp_{0.01} 32°

Other Data: Readily disproportionates to Dimethyl disulfide [CZS54-R](#) and Bis[(methylthio)methyl] disulfide [MHF37-L](#)

>>Derivative: S⁵-Oxide, (±)-

Synonym(s): Methyl (methylsulfinyl)methyl disulfide, 9CI

CAS Registry Number: 42474-27-1

Molecular Formula: C₃H₈OS₃

Molecular Weight: 156.294

Accurate Mass: 155.973725

Percentage Composition: C 23.05%; H 5.16%; O 10.24%; S 61.55%

Physical Description: Oil

Boiling Point: Bp_{0.04} 98°

Solubility: Sol. H₂O

>>Derivative: S⁵,S⁵-Dioxide

Synonym(s): Methyl (methylsulfonyl)methyl disulfide

CAS Registry Number: 42474-28-2

Molecular Formula: C₃H₈O₂S₃

Molecular Weight: 172.293

Accurate Mass: 171.96864

Percentage Composition: C 20.91%; H 4.68%; O 18.57%; S 55.83%

Physical Description: Sl. yellow oil

References:

- Block, E. *et al.*, *J.A.C.S.*, 1974, **96**, 3929-3944, (*S*⁵-oxides, synth, ir, pmr, ms)
Buttery, R.G. *et al.*, *J. Agric. Food Chem.*, 1976, **24**, 829-832, (*isol*)
Dumont, J.P. *et al.*, *Lait*, 1976, **56**, 595-599, (*isol*)
Dubs, P. *et al.*, *Helv. Chim. Acta*, 1978, **61**, 2351-2359, (*synth, ir, pmr, ms*)
Moir, M. *et al.*, *Phytochemistry*, 1980, **19**, 2201, (*isol, synth, spectra*)
Kubota, K. *et al.*, *Biosci., Biotechnol., Biochem.*, 1994, **58**, 644-646, (*isol, bibl*)