

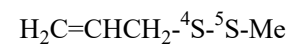


>>Entry Name: Methyl 2-propenyl disulfide

Synonym(s): Allyl methyl disulfide. 4,5-Dithia-1-hexene

CAS Registry Number: 2179-58-0

Related CAS Registry Numbers(s): 41865-22-9



Molecular Formula: C₄H₈S₂

Molecular Weight: 120.239

Accurate Mass: 120.00674

Percentage Composition: C 39.96%; H 6.71%; S 53.34%

Biological Source: Constit. of the essential oils of *Allium* spp.

Physical Description: Oil

Aldrich: W31270-3

>>Derivative: 4-Oxide

Synonym(s): S-Methyl 2-propene-1-sulfinothioate

CAS Registry Number: 3736-98-9

Molecular Formula: C₄H₈OS₂

Molecular Weight: 136.239

Accurate Mass: 136.001655

Percentage Composition: C 35.26%; H 5.92%; O 11.74%; S 47.07%

Biological Source: Constit. of *Allium* spp.

>>Derivative: 5-Oxide

Synonym(s): S-2-Propenyl methanesulfinothioate. Allyl methanethiosulfinate

CAS Registry Number: 104228-49-1

Molecular Formula: C₄H₈OS₂

Molecular Weight: 136.239

Accurate Mass: 136.001655

Percentage Composition: C 35.26%; H 5.92%; O 11.74%; S 47.07%

Biological Source: Constit. of *Allium* spp.

Physical Description: Oil

References:

Armitage, D.A. *et al.*, *J.C.S. Perkin 1*, 1972, 680, (*synth*)

Baechler, R.D. *et al.*, *Tet. Lett.*, 1978, 105, (*synth*)

Block, E. *et al.*, *J.A.C.S.*, 1986, **108**, 7045-7055, (*deriv, synth, pmr*)

Devlin, M.T. *et al.*, *J. Mol. Struct.*, 1990, **238**, 119, (*Raman, conformn*)

Block, E. *et al.*, *Pure Appl. Chem.*, 1993, **65**, 625-632, (*occur*)