



>>Entry Name: 3-(Methylthio)-1-propene, 9CI

Synonym(s): Allyl methyl sulfide, 8CI. Methyl 2-propenyl sulfide

CAS Registry Number: 10152-76-8

Related CAS Registry Numbers(s): 21892-75-1

$\text{H}_2\text{C}=\text{CHCH}_2\text{SMe}$

Molecular Formula: $\text{C}_4\text{H}_8\text{S}$

Molecular Weight: 88.173

Accurate Mass: 88.03467

Percentage Composition: C 54.49%; H 9.14%; S 36.37%

Biological Source: Constit. of *Allium* spp.

Physical Description: Oil

Boiling Point: Bp 91-93°

Density: d^{20}_4 0.877

Refractive Index: n^{20}_D 1.4712

Aldrich: A3420-1

>>Derivative: S-Oxide, (+)-form

Synonym(s): 3-(Methylsulfonyl)-1-propene, 9CI. Allyl methyl sulfoxide

CAS Registry Number: 21632-71-3

Molecular Formula: $\text{C}_4\text{H}_8\text{OS}$

Molecular Weight: 104.173

Accurate Mass: 104.029585

Percentage Composition: C 46.12%; H 7.74%; O 15.36%; S 30.78%

Optical Rotation: $[\alpha]^{24}_D$ +4.9 (c, 2.14 in EtOH)

>>Derivative: S,S-Dioxide

Synonym(s): 3-(Methylsulfonyl)-1-propene. Allyl methyl sulfone

Molecular Formula: $\text{C}_4\text{H}_8\text{O}_2\text{S}$

Molecular Weight: 120.172

Accurate Mass: 120.0245

Percentage Composition: C 39.98%; H 6.71%; O 26.63%; S 26.68%

Boiling Point: Bp₁ 135°

References:

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Obermeyer, J., *Ber.*, 1887, **20**, 2925, (synth)

Challenger, F. *et al.*, *Biochem. J.*, 1949, **44**, 89, (synth)

Axelrod, M. *et al.*, *J.A.C.S.*, 1968, **90**, 4835, (oxide, synth, pmr)

Baechler, R.D. *et al.*, *Tet. Lett.*, 1978, **2**, 105, (oxide, synth)

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