



>>Entry Name: Methyl methylsulfinylmethyl sulfide, 9CI

Synonym(s): Methyl methylthiomethyl sulfoxide. (Methylsulfinyl)(methylthio)methane

CAS Registry Number: 33577-16-1

Related CAS Registry Numbers(s): 95833-69-5

MeSOCH₂SMe

Molecular Formula: C₃H₈OS₂

Molecular Weight: 124.228

Accurate Mass: 124.001655

Percentage Composition: C 29.01%; H 6.49%; O 12.88%; S 51.62%

Use/Importance: Reagent for synth. of aldehydes. Li deriv. used to synthesise α-ketoesters

Aldrich: 17795-4

Fluka: 67865

Sigma: M9759

>>Variant: (R)-form

CAS Registry Number: 95833-70-8

Molecular Formula: C₃H₈OS₂

Molecular Weight: 124.228

Accurate Mass: 124.001655

Percentage Composition: C 29.01%; H 6.49%; O 12.88%; S 51.62%

Optical Rotation: [α]_D −29.7 (in Me₂CO) (40% ee)

>>Variant: (±)-form

Molecular Formula: C₃H₈OS₂

Molecular Weight: 124.228

Accurate Mass: 124.001655

Percentage Composition: C 29.01%; H 6.49%; O 12.88%; S 51.62%

Physical Description: Liq.

Boiling Point: Bp_{2.5} 92-93°

Refractive Index: n_D²⁰ 1.5487

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 879D

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **1**, 1418A

Ogura, K., *Bull. Chem. Soc. Jpn.*, 1972, **45**, 2203-2204, (*synth, ir, pmr, bibl*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 344, (*use*)

Bayer, E. *et al.*, *J. Chromatogr.*, 1985, **320**, 393-396, (*gc, resoln*)

Dunach, E. *et al.*, *Nouv. J. Chim.*, 1985, **9**, 1-3, (*R-form, synth*)

Lopez Sastre, J.A. *et al.*, *An. Quim.*, 1992, **88**, 508, (*asym synth*)