



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

ENTRY UNDER REVIEW

Synonym(s): 3-(Methylthio)propionaldehyde, 8CI. Methylmercaptoaldehyde. MMP. Methional. FEMA 2747

CAS Registry Number: 3268-49-3

MeSCH₂CH₂CHO

Molecular Formula: C₄H₈OS

Molecular Weight: 104.173

Accurate Mass: 104.029585

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

Use/Importance: Flavouring ingredient. Also a precursor in the biosynth. of ethylene and a reagent for triazoline synth.

Physical Description: Liq. with powerful onion/meat-like odour and meat/soup-like taste

Boiling Point: Bp 165-175°. Bp₁₄ 61°

Density: d²⁰ 1.14

Refractive Index: n_D²⁵ 1.4813

Hazard & Toxicity: LD₅₀ (rat, orl) 4400 mg/kg

Aldrich: W27470-4

Fluka: 67818

Sigma: M7879

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 7372-49-8

Physical Description: Cryst. (MeOH) or yellow-orange needles (EtOH)

Melting Point: Mp 122-123° (120.5°)

>>Derivative: Di-Me acetal

Synonym(s): 1,1-Dimethoxy-3-(methylthio)propane

CAS Registry Number: 13214-29-4

Molecular Formula: C₆H₁₄O₂S

Molecular Weight: 150.241

Accurate Mass: 150.07145

Percentage Composition: C 47.97%; H 9.39%; O 21.30%; S 21.34%

Boiling Point: Bp_{0.9} 73°

>>Derivative: Di-Et acetal

Synonym(s): 1,1-Diethoxy-3-(methylthio)propane

CAS Registry Number: 16630-61-8

Molecular Formula: C₈H₁₈O₂S

Molecular Weight: 178.295

Accurate Mass: 178.10275

Percentage Composition: C 53.89%; H 10.18%; O 17.95%; S 17.98%

Boiling Point: Bp₁₂ 91°. Bp_{0.7} 68-74°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 748B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 571A, (*ir*)

Catch, J.R. *et al.*, *J.C.S.*, 1947, 1609, (*synth*)

Pierson, E. *et al.*, *J.A.C.S.*, 1949, **70**, 1450, (*di-Et acetal*)

Mapson, L.W. *et al.*, *Biochem. J.*, 1969, **111**, 413-418, (*biosynth*)

Boustany, K.S. *et al.*, *Chimia*, 1969, **23**, 331-333, (*ir*)

Ichikawa, T. *et al.*, *J.O.C.*, 1970, **35**, 344-346, (*di-Me acetal*)

Courtrot, P. *et al.*, *C. R. Hebd. Seances Acad. Sci.*, 1975, **281**, 131-133, (*synth*)

Yoshifuji, M. *et al.*, *Chem. Lett.*, 1979, 723-726, (*di-Et acetal*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1875, (*occur, props*)