



>>Entry Name: 3-Methyl-2-butenal, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3-Methylcrotonaldehyde, 8CI. 3,3-Dimethylacrolein. Senecioaldehyde. Senecialdehyde. FEMA 3646

CAS Registry Number: 107-86-8

$(\text{H}_3\text{C})_2\text{C}=\text{CHCHO}$

Molecular Formula: $\text{C}_5\text{H}_8\text{O}$

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Biological Source: Isol. from *Tanacetum balsamita*

Use/Importance: Flavouring ingredient

Physical Description: Liq. with almond odour.

Boiling Point: Bp 132-133°

Density: d_4^{20} 0.872

Refractive Index: n_D^{20} 1.4526

Other Data: Readily oxidised

Aldrich: 30407-7

Fluka: 66260

>>Derivative: Phenylhydrazone

Physical Description: Reddish-violet cryst.

Melting Point: Mp 161-162°

>>Derivative: Semicarbazone

Physical Description: Cryst. (MeOH)

Melting Point: Mp 221-222°

>>Derivative: Di-Et acetal

Synonym(s): 1,1-Diethoxy-3-methyl-2-butene

CAS Registry Number: 1740-74-5

Molecular Formula: $\text{C}_9\text{H}_{18}\text{O}_2$

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Boiling Point: Bp 163-165°

Other Data: Easily dec.

References:

- Aldrich Library of ^{13}C and ^1H FT NMR Spectra*, 1992, **1**, 735B, (*nmr*)
- Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 559A, (*ir*)
- Wittig, G. *et al.*, *Tetrahedron, Suppl.*, No. 8, 1966, 347-358, (*synth*)
- Meyers, A.I. *et al.*, *J.A.C.S.*, 1969, **91**, 764-765, (*synth*)
- Pauling, H. *et al.*, *Helv. Chim. Acta*, 1976, **59**, 1233-1243, (*synth*)
- Cainelli, G. *et al.*, *J.A.C.S.*, 1976, **98**, 6737-6738, (*synth*)
- Erman, M.B. *et al.*, *Tet. Lett.*, 1976, 2981-2984, (*synth*)
- Cardillo, G. *et al.*, *Tetrahedron*, 1976, **32**, 107-108, (*synth*, *ir*, *pmr*)
- Schuda, P.F. *et al.*, *J.O.C.*, 1987, **52**, 1972-1979, (*synth*, *pmr*, *ir*)
- Klusener, P.A.A. *et al.*, *J.O.C.*, 1987, **52**, 5261-5266, (*synth*, *pmr*)
- Fenaroli's Handbook of Flavor Ingredients*, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 479
- Kubo, A. *et al.*, *J. Nat. Prod.*, 1995, **58**, 1565-1569, (*isol*)
- Encyclopedia of Food and Color Additives*, (ed. Burdock, G.A.), CRC Press, 1997, 1730-1731
- Schlosser, M. *et al.*, *Chem. Eur. J.*, 1998, **4**, 1738-1743, (*synth*, *pmr*)
- Picquet, M. *et al.*, *Eur. J. Org. Chem.*, 2000, 2361-2366, (*synth*, *ir*, *pmr*, *cmr*)
- Vani, P.V.S.N. *et al.*, *Synth. Commun.*, 2001, **31**, 219-224, (*synth*, *pmr*)
- Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., Van Nostrand Reinhold, 1979, 967