



>>Entry Name: 2-Heptenal, 9CI

ENTRY UNDER REVIEW

Synonym(s): FEMA 3165

CAS Registry Number: 2463-63-0

Related CAS Registry Numbers(s): 20810-22-4

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

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Biological Source: Isol. from soya bean oil (*Glycine max*)

Use/Importance: Flavouring constit. of many foods

Physical Description: Oil with pungent, green, somewhat fatty odour, pleasant only in extreme dilution

Density: d 0.86

Refractive Index: n_D^{20} 1.4491

>>Variant: (E)-form

CAS Registry Number: 18829-55-5

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Boiling Point: Bp 165-167°. Bp₁₅ 61-62°

Aldrich: 25176-3

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 2122-10-3

Melting Point: Mp 132-133°

>>Variant: (Z)-form

CAS Registry Number: 57266-86-1

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Boiling Point: Bp₁₆ 64-65°

>>Derivative: Di-Et acetal

Synonym(s): 1,1-Diethoxy-1-heptene

Molecular Formula: $\text{C}_{11}\text{H}_{22}\text{O}_2$

Molecular Weight: 186.294

Accurate Mass: 186.16198

Percentage Composition: C 70.92%; H 11.90%; O 17.18%

Boiling Point: Bp₁₅ 90-92°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 473A, (ir)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 737B, (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 560D, (ir)

Fujimaki, M. *et al.*, *Agric. Biol. Chem.*, 1965, **29**, 855, (isol)

Tadema, G. *et al.*, *CA*, 1976, **85**, 5141m, (synth)

Wada, M. *et al.*, *Chem. Lett.*, 1977, 345, (synth)

Yamamoto, K. *et al.*, *Synthesis*, 1977, 721, (synth, ir, pmr)

Bestmann, H.J. *et al.*, *Chem. Ber.*, 1982, **115**, 161, (synth)

Huang, Y.-Z. *et al.*, *J.O.C.*, 1987, **52**, 3558, (synth, ir, ms, pmr)

Ford, R.A. *et al.*, *Food Chem. Toxicol.*, 1988, **26**, 331, (rev, tox, E-form)

Fortes, C.C. *et al.*, *Synth. Commun.*, 1997, **27**, 3917-3941, (synth, ir, pmr, cmr, ms)