



>>Entry Name: 2,6-Dimethyl-5-heptenal, 9CI

ENTRY UNDER REVIEW

Synonym(s): Melonal. FEMA 2389

CAS Registry Number: 106-72-9

Type of Compound Code(s): VA1450

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

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}$

Molecular Weight: 140.225

Accurate Mass: 140.120115

Percentage Composition: C 77.09%; H 11.50%; O 11.41%

Biological Source: Constit. of the mollusc *Melibe leonina* and a pheromone of the ant *Lasius carnolicus*

Physical Description: Oil

Hazard & Toxicity: Skin and eye irritant

Aldrich: W23890-2

>>Variant: ($\pm$)-form

Type of Compound Code(s): WE2000

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}$

Molecular Weight: 140.225

Accurate Mass: 140.120115

Percentage Composition: C 77.09%; H 11.50%; O 11.41%

Use/Importance: Perfumery and flavouring ingredient

Physical Description: Liq. with melon-like odour and taste

Boiling Point: Bp_{100} 116-124°

>>Derivative: Oxime

CAS Registry Number: 22457-24-5

Molecular Formula: $\text{C}_9\text{H}_{17}\text{NO}$

Molecular Weight: 155.239

Accurate Mass: 155.131014

Percentage Composition: C 69.63%; H 11.04%; N 9.02%; O 10.31%

Boiling Point: $\text{Bp}_{0.9}$ 80-81°

>>Derivative: Semicarbazone

Melting Point: Mp 135°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 87°

>>Derivative: 1-Carboxylic acid

Synonym(s): 2,6-Dimethyl-5-heptenoic acid

Type of Compound Code(s): VA1500

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}_2$

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

Biological Source: Constit. of *Melibe leonina*

Physical Description: Oil

References:

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

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 561A, (ir)

Dominguez, X.A. *et al.*, *CA*, 1956, **50**, 8445, (synth)

Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1975, **13**, 793, (rev, tox)

Ayer, S.W. *et al.*, *Experientia*, 1983, **39**, 255-256, (isol)

Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DSD775

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992