



>>Entry Name: 3-Hexenal, 9CI

ENTRY UNDER REVIEW

CAS Registry Number: 4440-65-7

Extra CAS Registry Numbers(s): 1335-39-3

$\text{H}_3\text{CCH}_2\text{CH}=\text{CHCH}_2\text{CHO}$

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}$

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

>>Variant: (*E*)-form

CAS Registry Number: 69112-21-6

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}$

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

Boiling Point: Bp₃₆ 51.5-52.5°. Bp₂₀ 35°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 99-101°

>>Derivative: Semicarbazone

Melting Point: Mp 133-134°

>>Variant: (*Z*)-form

Synonym(s): FEMA 2561

CAS Registry Number: 6789-80-6

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}$

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

Biological Source: Constit. of cistus leaf oil. Also present in tea, tomatoes and cucumber

Use/Importance: Used in perfumery. Flavouring ingredient

Physical Description: Liq. with a powerful, deep-green, leafy odour

Boiling Point: Bp₇₃₀ 120°. Bp₂₀ 36°

Solubility: Sl. sol. H_2O , sol. EtOH

Density: d_4^{22} 0.853

Refractive Index: n_D^{22} 1.4300

Hazard & Toxicity: LD₅₀ (rat, orl) 1560 mg/kg

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 2121-99-5

Melting Point: Mp 99.5-101°. Mp 102.3-103.1°

>>Derivative: Semicarbazone

Melting Point: Mp 128-130°

References:

Winter, M. *et al.*, *Helv. Chim. Acta*, 1962, **45**, 2567, (*synth*)

Ford, R.A. *et al.*, *Food Chem. Toxicol.*, 1988, **26**, 343, (*rev, tox, E-form*)

Hatanaka, A. *et al.*, *Z. Naturforsch., C*, 1992, **47**, 183, (*synth, pmr, cmr*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 333

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1301-1302