>>**Entry Name: 3-Hexenal,** 9CI
ENTRY UNDER REVIEW

CAS Registry Number: 4440-65-7
Extra CAS Registry Numbers(s): 1335-39-3
$H_3CCH_2CH=CHCH_2CHO$

Molecular Formula: $C_6H_{10}O$
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: $C_6H_{10}O$
Molecular Weight: 98.144
Accurate Mass: 98.073165
Percentage Composition: C 73.43%; H 10.27%; O 16.30%
Boiling Point: Bp_{36} 51.5-52.5°. Bp_{20} 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: $C_6H_{10}O$
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: Bp_{730} 120°. Bp_{20} 36°
Solubility: Sl. sol. H_2O, sol. EtOH
Density: d_4^{22}0.853
Refractive Index: n_D^{22} 1.4300
Hazard & Toxicity: LD_{50} (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