



>>Entry Name: 2-Hexenal, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3-Propylacrolein. FEMA 2560

CAS Registry Number: 505-57-7

Related CAS Registry Numbers(s): 54306-00-2

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

$\text{H}_3\text{CCH}_2\text{CH}_2\text{CH}=\text{CHCHO}$

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 many foods, hornbeam leaves, and of scent gland of many bugs, e.g., *Pternistria bispina*; alarm pheromone of e.g. *Cimex lectularius*

Hazard & Toxicity: LD₅₀ (mus, ipr) 290 mg/kg

>>Variant: (E)-form

Synonym(s): Leaf aldehyde

CAS Registry Number: 6728-26-3

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%

Use/Importance: Used in perfumery and flavourings

Physical Description: Liq. with sharp herbal pungency, apple-like in high dilution

Boiling Point: Bp 146-147°. Bp₁₂ 43°

Refractive Index: n_D²⁰ 1.4480

Hazard & Toxicity: Peroxidizable. Skin irritant. LD₅₀ (rat, orl) 780 mg/kg. LD₅₀ (rbt, skn) 600 mg/kg

Aldrich: 13265-9

Fluka: 53000

Sigma: H7383

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 2122-02-3

Physical Description: Red needles

Melting Point: Mp 147°

>>Derivative: Semicarbazone

Physical Description: Cryst. (MeOH)

Melting Point: Mp 179°

>>Derivative: Di-Et acetal

Synonym(s): 1,1-Diethoxy-2-hexene

CAS Registry Number: 67746-30-9

Molecular Formula: $\text{C}_{10}\text{H}_{20}\text{O}_2$

Molecular Weight: 172.267

Accurate Mass: 172.14633

Percentage Composition: C 69.72%; H 11.70%; O 18.58%

Boiling Point: Bp₅₅ 95-98°

Density: d 0.85

Refractive Index: n_D²⁰ 1.4210