



>>Entry Name: Octanal, 9CI

Synonym(s): Caprylaldehyde. Caprylic aldehyde. Octyl aldehyde. FEMA 2797

CAS Registry Number: 124-13-0

$\text{H}_3\text{C}(\text{CH}_2)_6\text{CHO}$

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}$

Molecular Weight: 128.214

Accurate Mass: 128.120115

Percentage Composition: C 74.94%; H 12.58%; O 12.48%

Biological Source: Isol. from various citrus peel oils. Also present in cadamon, coriander, caraway and other herbs

Use/Importance: Flavouring agent, used in eau-de-cologne and artificial citrus formulations

Physical Description: Liq.

Boiling Point: Bp 163.4°. Bp₂₀ 72°

Density: d_4^{20} 0.82

Refractive Index: n_D^{26} 1.4167

Hazard & Toxicity: Flammable. Skin and eye irritant. LD₅₀ (rat, orl) 5630 mg/kg

Aldrich: O-560-8

Fluka: 21630

Sigma: O7128

Supelco: S48-2797

>>Derivative: Oxime

CAS Registry Number: 929-55-5

Molecular Formula: $\text{C}_8\text{H}_{17}\text{NO}$

Molecular Weight: 143.228

Accurate Mass: 143.131014

Percentage Composition: C 67.09%; H 11.96%; N 9.78%; O 11.17%

Physical Description: Cryst. (petrol or EtOH aq.)

Melting Point: Mp 60°

Boiling Point: Bp₉ 112°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 1726-77-8

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 106°

Rare Chemicals Library: S64807-8

>>Derivative: Semicarbazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 101°

>>Derivative: Di-Me acetal

Synonym(s): 1,1-Dimethoxyoctane, 9CI

CAS Registry Number: 10022-28-3

Molecular Formula: $\text{C}_{10}\text{H}_{22}\text{O}_2$

Molecular Weight: 174.283

Accurate Mass: 174.16198

Percentage Composition: C 68.92%; H 12.72%; O 18.36%

Physical Description: Liq.

Boiling Point: Bp₂₀ 88-89°

>>Derivative: Di-Et acetal

Synonym(s): 1,1-Diethoxyoctane, 9CI