



>>Entry Name: Pentanal, 9CI

ENTRY UNDER REVIEW

Synonym(s): *n*-Valeraldehyde, 8CI. Valeric aldehyde. FEMA 3098

CAS Registry Number: 110-62-3

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

Molecular Formula: $\text{C}_5\text{H}_{10}\text{O}$

Molecular Weight: 86.133

Accurate Mass: 86.073165

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

Biological Source: Found in olive oil and several essential oils. Also present in Bantu beer, plum brandy, cardamon, coriander leaf, rice, Bourbon vanilla, clary sage, cooked shrimps, seaclogs, apple and banana, sweet cherry, blackcurrant and other foods

Use/Importance: Used to make flavouring compounds and resins

Physical Description: Liq.

Melting Point: Fp -92°

Boiling Point: Bp $102.5-103^\circ$

Density: d_4^{20} 0.811

Refractive Index: n_D^{20} 1.3947

Hazard & Toxicity: Highly flammable, fl. p. 12° , autoignition temp. 222° . Eye, skin and respiratory tract irritant. LD₅₀ (rat, orl) 3200 mg/kg. LD₅₀ (rbt, skn) 4857 mg/kg

Aldrich: 11013-2

Fluka: 94512

Sigma: V2378

>>Derivative: Oxime

CAS Registry Number: 628-79-5

Molecular Formula: $\text{C}_5\text{H}_{11}\text{NO}$

Molecular Weight: 101.148

Accurate Mass: 101.084064

Percentage Composition: C 59.37%; H 10.96%; N 13.85%; O 15.82%

Physical Description: Cryst.

Melting Point: Mp 52°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 2057-84-3

Physical Description: Yellow cryst.

Melting Point: Mp $106-107^\circ$

Aldrich: 42957-0

Supelco: 44-2834

>>Derivative: Di-Me acetal

Synonym(s): 1,1-Dimethoxypentane

CAS Registry Number: 26450-58-8

Molecular Formula: $\text{C}_7\text{H}_{16}\text{O}_2$

Molecular Weight: 132.202

Accurate Mass: 132.11503

Percentage Composition: C 63.60%; H 12.20%; O 24.20%

Physical Description: Liq.

Boiling Point: Bp $120-129^\circ$

>>Derivative: Di-Et acetal

Synonym(s): 1,1-Diethoxypentane

CAS Registry Number: 3658-79-5

Molecular Formula: $\text{C}_9\text{H}_{20}\text{O}_2$

Molecular Weight: 160.256

Accurate Mass: 160.14633

Percentage Composition: C 67.45%; H 12.58%; O 19.97%

Biological Source: Volatile component of strawberries and other fruits

Physical Description: Liq.

Boiling Point: Bp $162.5-163.5^\circ$. Bp₁₂ 59°

Density: d_4^{22} 0.829

Refractive Index: n