



>>Entry Name: 1-Heptanol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Heptyl alcohol, 8CI. FEMA 2548

CAS Registry Number: 111-70-6

Extra CAS Registry Numbers(s): 53535-33-4

$\text{H}_3\text{C}(\text{CH}_2)_5\text{CH}_2\text{OH}$

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

Molecular Weight: 116.203

Accurate Mass: 116.120115

Percentage Composition: C 72.35%; H 13.88%; O 13.77%

Biological Source: Found in a few essential oils, e.g. *Rosa rugosa* and the fungus *Coriolus sanguineus*

Use/Importance: Simple esters used in flavourings and perfumery. Flavouring ingredient

Physical Description: Liq. with pungent spicy taste

Melting Point: Fp -34.1°

Boiling Point: Bp 176.3° . Bp₁₅ 78-79°

Density: d_4^{20} 0.82

Refractive Index: n_D^{20} 1.4241

Hazard & Toxicity: LD₅₀ (rat, orl) 500 mg/kg. Fl. p. 63/74°

Aldrich: H280-5

Fluka: 51778

Sigma: H6129

>>Derivative: Formyl

Synonym(s): Heptyl formate. FEMA 2552

CAS Registry Number: 112-23-2

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_2$

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Use/Importance: Used in perfumery and food flavouring

Boiling Point: Bp 178°

Density: d 0.88

>>Derivative: Ac

Synonym(s): Heptyl acetate. Acetate C7. FEMA 2547

CAS Registry Number: 112-06-1

Molecular Formula: $\text{C}_9\text{H}_{18}\text{O}_2$

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Use/Importance: Perfumery ingredient

Physical Description: Liq. with sweet apricot-like taste

Melting Point: Fp -50°

Boiling Point: Bp 191.5°

Density: d_4^{15} 0.88

Refractive Index: n_D^{20} 1.4150

Hazard & Toxicity: Eye, skin and mucous membrane irritant

Aldrich: W25470-3

Rare Chemicals Library: S43171-0

Sigma: H0755