



>>Entry Name: 3,5,5-Trimethyl-1-hexanol, 9CI, 8CI

ENTRY UNDER REVIEW

Synonym(s): Inonanol. FEMA 3324

CAS Registry Number: 3452-97-9

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

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

Molecular Weight: 144.256

Accurate Mass: 144.151415

Percentage Composition: C 74.94%; H 13.97%; O 11.09%

Aldrich: 28948-5

>>Variant: ($\pm$)-form

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

Molecular Weight: 144.256

Accurate Mass: 144.151415

Percentage Composition: C 74.94%; H 13.97%; O 11.09%

Source/Synthesis: Prepd. comly. from 2,5-Dimethyl-1,5-hexadiene [CZV16-W](#) by oxo synth. followed by redn.

Use/Importance: Perfumery and flavouring ingredient

Physical Description: Liq. with a strong only-herbaceous odour

Boiling Point: Bp 193-194°. Bp₁₅₀ 142°

Solubility: Sol. EtOH, Me₂CO, Et₂O

Density: d²⁰ 0.825

Refractive Index: n_D²⁰ 1.4352

Hazard & Toxicity: Fl. p. 93° (oc)

>>Derivative: Ac

Synonym(s): 3,5,5-Trimethylhexyl acetate. Inonyl acetate. Isononyl acetate

CAS Registry Number: 58430-94-7

Molecular Formula: $\text{C}_{11}\text{H}_{22}\text{O}_2$

Molecular Weight: 186.294

Accurate Mass: 186.16198

Percentage Composition: C 70.92%; H 11.90%; O 17.18%

Use/Importance: Used in perfumery formulations

Physical Description: Liq. with woody/fruity odour

Boiling Point: Bp 209°

Hazard & Toxicity: LD₅₀ (rat, orl) 4250 mg/kg

Rare Chemicals Library: S52853-6

>>Derivative: 2-Propenoyl

CAS Registry Number: 2664-55-3

Molecular Formula: $\text{C}_{12}\text{H}_{22}\text{O}_2$

Molecular Weight: 198.305

Accurate Mass: 198.16198

Percentage Composition: C 72.68%; H 11.18%; O 16.14%

Melting Point: Mp -34°

Boiling Point: Bp_{0.4} 55°

Refractive Index: n_D²⁰ 1.4370

Aldrich: 42402-1

>>Derivative: 3,5-Dinitrobenzoyl

Melting Point: Mp 62°

References: