>>**Entry Name: 3,5,5-Trimethyl-1-hexanol,** 9Cl, 8Cl
ENTRY UNDER REVIEW
Synonym(s): Inonanol. FEMA 3324

CAS Registry Number: 3452-97-9
$(H_3C)_3CCH_2CH(CH_3)CH_2CH_2OH$

Molecular Formula: $C_9H_{20}O$
Molecular Weight: 144.256
Accurate Mass: 144.151415
Percentage Composition: C 74.94%; H 13.97%; O 11.09%

Aldrich: 28948-5

>>**Variant:** (±)-form

Molecular Formula: $C_9H_{20}O$
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°. Bp_{150} 142°
Solubility: Sol. EtOH, Me_2CO, Et_2O
Density: d^{20} 0.825
Refractive Index: n_D^{20} 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: $C_{11}H_{22}O_2$
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: LD_{50} (rat, orl) 4250 mg/kg

Rare Chemicals Library: S52853-6

>>**Derivative:** 2-Propenoyl

CAS Registry Number: 2664-55-3
Molecular Formula: $C_{12}H_{22}O_2$
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_D^{20} 1.4370
Aldrich: 42402-1

>>**Derivative:** 3,5-Dinitrobenzoyl

Melting Point: Mp 62°

References: