



>>Entry Name: 1-Undecanol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Alcohol C11. Undecylic alcohol. FEMA 3097

CAS Registry Number: 112-42-5

Extra CAS Registry Numbers(s): 30207-98-8

$\text{H}_3\text{C}(\text{CH}_2)_9\text{CH}_2\text{OH}$

Molecular Formula:  $\text{C}_{11}\text{H}_{24}\text{O}$

Molecular Weight: 172.31

Accurate Mass: 172.182715

Percentage Composition: C 76.68%; H 14.04%; O 9.29%

Biological Source: Isol. from hop oil (*Humulus lupulus*). Acetate possibly a minor component of the sex pheromone of the female fruit tree leaf roller *Archips argyrospilus*

Use/Importance: Perfumery ingredient, flavouring agent

Physical Description: Liq. or cryst., with floral citrus-like odour and fatty flavour

Melting Point: Mp 19° (16.5°)

Boiling Point: Bp<sub>15</sub> 131°. Bp<sub>6</sub> 123-125°

Density:  $d_4^{23}$  0.833

Refractive Index:  $n_D^{23}$  1.4392

Hazard & Toxicity: Skin irritant. LD<sub>50</sub> (rat, orl) 3000 mg/kg

Aldrich: U100-1

Fluka: 94059

Sigma: U4376

>>Derivative: Ac

Synonym(s): Undecyl acetate. Acetate C11

CAS Registry Number: 1731-81-3

Molecular Formula:  $\text{C}_{13}\text{H}_{26}\text{O}_2$

Molecular Weight: 214.347

Accurate Mass: 214.19328

Percentage Composition: C 72.85%; H 12.23%; O 14.93%

Use/Importance: Perfumery ingredient

Boiling Point: Bp<sub>5</sub> 119°

Sigma: U4126

>>Derivative: Benzoyl

CAS Registry Number: 6316-30-9

Molecular Formula:  $\text{C}_{18}\text{H}_{28}\text{O}_2$

Molecular Weight: 276.418

Accurate Mass: 276.20893

Percentage Composition: C 78.21%; H 10.21%; O 11.58%

Physical Description: Liq.

Refractive Index:  $n_D^{20}$  1.4841

>>Derivative: 4-Nitrobenzoyl

CAS Registry Number: 93094-34-9

Melting Point: Mp 29.2°

References: