



>>Entry Name: 2-Undecanol

ENTRY UNDER REVIEW

Synonym(s): FEMA 3246

CAS Registry Number: 1653-30-1

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

$\text{H}_3\text{C}(\text{CH}_2)_8\text{CH}(\text{OH})\text{CH}_3$

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%

Use/Importance: Flavouring agent

Hazard & Toxicity: Fl. p. 113° (oc)

Aldrich: U120-6

Rare Chemicals Library: S41037-3

Sigma: U5003

>>Variant: (R)-form

CAS Registry Number: 85617-06-7

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 leaf oil of *Litsea odorifera*, rue (*Ruta graveolens*) and a few other sources

Boiling Point: Bp 231-233°

>>Variant: (S)-form

CAS Registry Number: 85617-05-6

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 cocoa butter and coconut

Melting Point: Mp 12°

Boiling Point: Bp₂₀ 128°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +8.11$ (EtOH). $[\alpha]_{\text{D}}^{20} +10.29$ (C_6H_6)

>>Derivative: Ac

CAS Registry Number: 14936-67-5

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%

Boiling Point: Bp₁₅ 84°

>>Derivative: Benzoyl

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%

Boiling Point: Bp_{3.5} 159°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +27.55$

>>Derivative: Hydrogen phthalate

Melting Point: Mp 31-32°

Optical Rotation: $[\alpha]_{\text{D}} +37.3$ (CHCl_3). $[\alpha]_{\text{D}} +44.3$ (EtOH)