



>>Entry Name: Undecanoic acid, 9CI, 8CI

ENTRY UNDER REVIEW

Synonym(s): Decane-1-carboxylic acid. Hendecanoic acid. Undecylic acid. FEMA 3245

CAS Registry Number: 112-37-8

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

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%

Biological Source: Constit. of numerous plant spp.

Physical Description: Cryst. (AcOH aq.)

Melting Point: Mp 28.2-28.6°

Boiling Point: Bp₁₀₀ 212.5°. Bp₁₅ 164°

Solubility: Insol. H_2O ; sol. EtOH, CHCl_3 , Me_2CO , C_6H_6

Hazard & Toxicity: Skin irritant. LD₅₀ (mus, ivn) 140 mg/kg

Aldrich: W32450-7

Fluka: 94090

Sigma: U5503

>>Derivative: Me ester

CAS Registry Number: 1731-86-8

Molecular Formula: $\text{C}_{12}\text{H}_{24}\text{O}_2$

Molecular Weight: 200.32

Accurate Mass: 200.17763

Percentage Composition: C 71.95%; H 12.08%; O 15.97%

Use/Importance: Used in perfumery

Physical Description: Liq.

Boiling Point: Bp_{9.5} 123° (lit. gives a pressure range). Bp₁ 70-72°

Aldrich: 29941-3

Fluka: 94120

Sigma: U0250

Supelco: R42-0115

>>Derivative: Et ester

Synonym(s): FEMA 3492

CAS Registry Number: 627-90-7

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: Used in perfumery

Physical Description: Liq.

Boiling Point: Bp₂₀ 140°

Aldrich: W34920-8

Sigma: U3876

Supelco: R30-0435

>>Derivative: Vinyl ester

CAS Registry Number: 20690-63-5

Molecular Formula: $\text{C}_{13}\text{H}_{24}\text{O}_2$

Molecular Weight: 212.331

Accurate Mass: 212.17763

Percentage Composition: C 73.54%; H 11.39%; O 15.07%

Physical Description: Liq.

Boiling Point: Bp₁₀ 125°

Density: d₂₀ 0.882

Refractive Index: n_D²⁰ 1.4355

Other Data: Q/e values for radical polym., Q 0.056, e -0.84