



>>Entry Name: Nonanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Nonoic acid. Pelargonic acid. Octane-1-carboxylic acid. Nonylic acid. FEMA 2784

CAS Registry Number: 112-05-0

Related CAS Registry Numbers(s): 14047-60-0

$\text{H}_3\text{C}(\text{CH}_2)_7\text{COOH}$

Molecular Formula: $\text{C}_9\text{H}_{18}\text{O}_2$

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Biological Source: Occurs as esters in oil of pelargonium. Acid isol. from *Ajania*, *Rubus*, *Rhamnus*, *Paulownia*, *Artemisia* spp., numerous other plant sources and human skin

Use/Importance: Simple esters used as flavouring ingredients

Biological Use/Importance: Acts as bactericide and fungicide. Used in snail repellents. Herbicide plant growth regulator

Physical Description: Oily, irritant liq. with characteristic odour and a correspondant unpleasant taste

Melting Point: Mp 15°. Fp 12.24°

Boiling Point: Bp 255°. Bp₁ 98.9°

Density: d_4^{20} 0.9052

pKa Value: $\text{p}K_a$ 4.95

Refractive Index: n_D^{20} 1.4309

Other Data: Spar. steam-volatile

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (mus, orl) 15000 mg/kg

Aldrich: N2990-2

Fluka: 76343

Sigma: N8253

>>Derivative: NH_4 salt

CAS Registry Number: 63718-65-0

Physical Description: Solid (H_2O)

Melting Point: Mp 115°

>>Derivative: Me ester

Synonym(s): FEMA 2724

CAS Registry Number: 1731-84-6

Molecular Formula: $\text{C}_{10}\text{H}_{20}\text{O}_2$

Molecular Weight: 172.267

Accurate Mass: 172.14633

Percentage Composition: C 69.72%; H 11.70%; O 18.58%

Biological Source: Isol. from *Cistus*, *Hyssopus* and *Pinus* spp., and from civet, cloves, hops, tobacco, vanilla and certain wines

Physical Description: Liq. with a wine and coconut-like odour

Melting Point: Mp -35°

Boiling Point: Bp 213.5-214°. Bp₈ 88-91°

Solubility: Insol. H_2O sol. EtOH, Et₂O

Density: d^{18} 0.88

Refractive Index: n_D^{25} 1.4302

Aldrich: 24589-5

Fluka: 76370

Rare Chemicals Library: S57096-6

Sigma: N5627

>>Derivative: Et ester

Synonym(s): FEMA 2447

CAS Registry Number: 123-29-5