



>>Entry Name: Octanoic acid, 9CI, INN, USAN

Synonym(s): Heptane-1-carboxylic acid. Caprylic acid. Octoic acid. *n*-Octylic acid. FEMA 2799

CAS Registry Number: 124-07-2

Related CAS Registry Numbers(s): 557-09-5 5461-06-3

$\text{H}_3\text{C}(\text{CH}_2)_6\text{COOH}$

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_2$

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Biological Source: Widespread in plant oils, free and as glycerides. Manuf. by oxo reaction from heptene

Use/Importance: Used in perfume and dye manuf. Simple esters have flavour use. Antifungal agent. Used as a soln. in CHCl_3 /butanol for extraction-separation of Co, Fe, Rh, Ti, Al, Ga, In. Used in hydraulic fluids, flotation agents and as wood preservative

Physical Description: Liq. or cryst. with burning, rancid taste

Melting Point: Mp 16°

Boiling Point: Bp 239.7°. Bp₁₀ 124°

Solubility: Sol. alkalis, EtOH, CHCl_3 ; spar. sol. hot H_2O

Density: d_4^{20} 0.91

pKa Value: $\text{p}K_a$ 4.89 (25°)

Refractive Index: n_D^{20} 1.4335

Calculated Log P Data: Log P 2.94 (calc)

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) approx. 10000 mg/kg. Fl. p. >107°

Aldrich: W27992-7

Fluka: 21650

Sigma: C3000

>>Derivative: Me ester

Synonym(s): Methyl octanoate. Methyl caprylate. FEMA 2728

CAS Registry Number: 111-11-5

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: Present in many fruits, e.g. apple, apricot, grapes, blackberry, cherimoya etc.

Use/Importance: Flavouring agent

Physical Description: Oil with oily, somewhat orange-like taste

Boiling Point: Bp 193-194°. Bp₁₅ 83°

Density: d_4^{20} 0.88

Refractive Index: n_D^{20} 1.4180

Aldrich: W27280-9

Fluka: 21720

Sigma: C3375

>>Derivative: Et ester

Synonym(s): Ethyl octanoate. Ethyl caprylate. FEMA 2449

CAS Registry Number: 106-32-1

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%

Source/Synthesis: Constit. of plant oils. Also present in Swiss cheese, Camembert cheese, wheat bread, port wine, plum brandy, sparkling wine, apple, apricot, banana, cherry, orange, grapefruit plum and other fruits

Use/Importance: Used in many fruit flavourings

Physical Description: Liq. with fruity/flowery odour

Boiling Point: Bp 207°

Refractive Index: n_D^{20} 1.4178