



>>Entry Name: Pentanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Valeric acid, 8CI. FEMA 3101

CAS Registry Number: 109-52-4

Related CAS Registry Numbers(s): 6106-41-8

$\text{H}_3\text{CCH}_2\text{CH}_2\text{CH}_2\text{COOH}$

Molecular Formula: $\text{C}_5\text{H}_{10}\text{O}_2$

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Biological Source: Minor constit. of biological systems e.g. yeast fat, some plant oils. Earlier reported isols. were mostly of 3-Methylbutanoic acid [BZM14-Q](#)

Use/Importance: Antihypertensive agent. Tranquilliser. Important intermediate in the manuf. of perfumes. Flavouring agent

Physical Description: Liq. with unpleasant rancid odour

Melting Point: Fp -34.5°

Boiling Point: Bp 186° . Bp₁₅ $86-88^\circ$

Solubility: Sol. EtOH, Et₂O; spar. sol. H₂O

Density: d_4^{20} 0.9459

pKa Value: pK_a 4.81

Refractive Index: n_D^{23} 1.4075

Calculated Log P Data: Log P 1.35 (calc)

Hazard & Toxicity: Fl. p. 89° , autoignition temp. 400° . Corrosive and irritating to skin, eyes and mucous membranes. LD₅₀ (mus, orl) 600 mg/kg

Aldrich: W31010-7

Fluka: 94530

Sigma: V9759

Supelco: R42-0050

>>Derivative: Benzylamine salt

Physical Description: Cryst.

Melting Point: Mp $56-57^\circ$

>>Derivative: Me ester

Synonym(s): Methyl pentanoate. Methyl valerate. FEMA 2752

CAS Registry Number: 624-24-8

Molecular Formula: $\text{C}_6\text{H}_{12}\text{O}_2$

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Biological Source: Found in varous fruits

Use/Importance: Flavouring agent

Physical Description: Liq. with apple- and pineapple-like taste and odour at low cone

Boiling Point: Bp 127.3° . Bp₁₃₀ $74-79^\circ$

Hazard & Toxicity: Flammable, fl. p. $<25^\circ$

Aldrich: W27520-4

Fluka: 94562

Sigma: V0880

>>Derivative: Et ester

Synonym(s): Ethyl pentanoate. Ethyl valerate. FEMA 2462

CAS Registry Number: 539-82-2

Molecular Formula: $\text{C}_7\text{H}_{14}\text{O}_2$

Molecular Weight: 130.186

Accurate Mass: 130.09938

Percentage Composition: C 64.58%; H 10.84%; O 24.58%

Biological Source: Found in various fruits

Use/Importance: Flavouring agent

Physical Description: Liq. with fruity, apple-like odour

Boiling Point: Bp 145.1°

Density: d_4^{20} 0.87

Refractive Index: n