



>>Entry Name: Propanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Propionic acid. Metacetic acid. Ethanoic acid

CAS Registry Number: 79-09-4

Related CAS Registry Numbers(s): 72-03-7 137-40-6 4075-81-4 16674-79-6 17448-65-6

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

Molecular Formula: $\text{C}_3\text{H}_6\text{O}_2$

Molecular Weight: 74.079

Accurate Mass: 74.03678

Percentage Composition: C 48.64%; H 8.16%; O 43.20%

Biological Source: Volatile component of human vaginal secretions. Gut flora metabolite, found in faeces. Manuf. by oxidation of naphtha or butane

Use/Importance: Preservative used esp. in bread and grain mould inhibitors. Also used in cosmetics and pharmaceuticals. Also used in cellulose propionate manuf. Antifungal agent (and salts)

Physical Description: Liq. with acrid odour

Melting Point: Mp -21.5°

Boiling Point: Bp 141.1° . Bp₁₀ 39.7°

Solubility: Misc. H_2O

Density: d_{15}^{15} 0.999

Other Data: Simple esters used as flavouring agents

Hazard & Toxicity: Corrosive and mod. irritating to skin, eyes and respiratory tract. LD₅₀ (rat, orl) 3500 mg/kg. OES: long-term 10 ppm; short-term 15 ppm

Aldrich: W29240-0

Fluka: 81910

Sigma: P5561

Supelco: 4-7855

>>Derivative: NH_4 salt

CAS Registry Number: 17496-08-1

Physical Description: V. hygroscopic cryst.

Melting Point: Mp 45°

>>Derivative: K salt

CAS Registry Number: 327-62-8

Physical Description: Plates + $1\text{H}_2\text{O}$ (EtOH aq.)

Melting Point: Mp 300°

>>Derivative: Me ester

Synonym(s): Methyl propionate

CAS Registry Number: 554-12-1

Molecular Formula: $\text{C}_4\text{H}_8\text{O}_2$

Molecular Weight: 88.106

Accurate Mass: 88.05243

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

Physical Description: Liq.

Boiling Point: Bp 79.7°

Density: d_4^0 0.939

Refractive Index: n_D^{19} 1.3770

Hazard & Toxicity: Highly flammable, fl. p. -2° , autoignition temp. 469° . Skin irritant

Aldrich: 10925-8

Fluka: 81988

Sigma: P1282