



>>Entry Name: 4-Oxopentanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Levulinic acid, 8CI. 3-Acetylpropionic acid. FEMA 2627

CAS Registry Number: 123-76-2

Related CAS Registry Numbers(s): 591-64-0

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

Molecular Formula: $\text{C}_5\text{H}_8\text{O}_3$

Molecular Weight: 116.116

Accurate Mass: 116.047345

Percentage Composition: C 51.72%; H 6.94%; O 41.34%

Biological Source: Found in sphagnum peat, wood waste, tobacco, bagasse, beet, caramel etc. Also prod. by *Litchi chinensis*, *Basella rubra* and *Phyllophora* spp. Obt. by the action of dil. acids on carbohydrates, e.g. sucrose, glucose, starch

Use/Importance: Used to make antacids, cathartics and shampoos, nylon, synthetic rubber, plastics and medicines. Flavour ingredient. Reagent for cleavage of oximes and 2, 4-dinitrophenylhydrazones

Physical Description: Plates or leaflets with tart, whisky taste

Melting Point: Mp 33.5°

Boiling Point: Bp 245°. Bp₁₄ 143-147°

Solubility: V. sol. H_2O , EtOH, Et₂O; insol. hydrocarbons

pKa Value: pK_a 4.62

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 1850 mg/kg

Aldrich: W26270-6

Fluka: 61380

Sigma: L0626

>>Derivative: Ca salt (2:1)

Synonym(s): Calcium levulinate, USAN

CAS Registry Number: 5743-49-7

Use/Importance: Calcium replenisher

Fluka: 61385

Sigma: L7020

>>Derivative: Me ester

CAS Registry Number: 624-45-3

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_3$

Molecular Weight: 130.143

Accurate Mass: 130.062995

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

Physical Description: Liq.

Boiling Point: Bp 196°. Bp_{0.1} 36°

Fluka: 61405

>>Derivative: Me ester, semicarbazone

Physical Description: Cryst.

Melting Point: Mp 142-143°

>>Derivative: Et ester

CAS Registry Number: 539-88-8

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_3$

Molecular Weight: 144.17

Accurate Mass: 144.078645

Percentage Composition: C 58.32%; H 8.39%; O 33.29%

Physical Description: Liq.

Boiling Point: Bp 199-201°. Bp_{0.1} 38°

Refractive Index: n_D²⁰ 1.4220

Aldrich: W24420-1

Fluka: 61395

Rare Chemicals Library: S3614-6

Sigma: L3008