



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

Synonym(s): Succinaldehydic acid, 8CI. Succinic semialdehyde. 3-Formylpropionic acid. γ -Oxobutanoic acid

CAS Registry Number: 692-29-5

OHCCH2CH2COOH

Molecular Formula: $C_4H_6O_3$

Molecular Weight: 102.09

Accurate Mass: 102.031695

Percentage Composition: C 47.06%; H 5.92%; O 47.02%

Biological Source: Found in *Proteus vulgaris*, and in mouse brains

Use/Importance: Has anaesthetic props.

Physical Description: Oil with rancid odour

Boiling Point: Bp_{14} 134-136°

Solubility: Sol. H_2O , EtOH, Et_2O , C_6H_6

Other Data: Steam-volatile

Hazard & Toxicity: LD_{50} (mus, ipr) 1900 mg/kg

Aldrich: 28718-0

Fluka: 14075

Sigma: S1505

>>Derivative: Trimer

Synonym(s): 1,3,5-Trioxane-2,4,6-tripropanoic acid. 1,3,5-Tris-(β -carboxyethyl)-s-trioxane

CAS Registry Number: 26817-25-4

Molecular Formula: $C_{12}H_{18}O_9$

Molecular Weight: 306.269

Accurate Mass: 306.095085

Percentage Composition: C 47.06%; H 5.92%; O 47.02%

Physical Description: Prisms

Melting Point: Mp 147°

Boiling Point: Bp_{14} 134-136°

Solubility: Sl. sol. Et_2O , EtOAc, aq. Na_2CO_3

Other Data: On dist. $\rightarrow$ monomer

>>Derivative: Oxime

Molecular Formula: $C_4H_7NO_3$

Molecular Weight: 117.104

Accurate Mass: 117.042594

Percentage Composition: C 41.03%; H 6.02%; N 11.96%; O 40.99%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 102-103° (155)

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 4093-65-6

Physical Description: Yellow cryst.

Melting Point: Mp 201°

>>Derivative: Semicarbazone

Physical Description: Prisms or needles (H_2O)

Melting Point: Mp 190-191 dec.°

>>Derivative: Me ester

CAS Registry Number: 13865-19-5

Molecular Formula: $C_5H_8O_3$

Molecular Weight: 116.116

Accurate Mass: 116.047345

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

Physical Description: Oil

Boiling Point: Bp_{15} 69-71°