



>>Entry Name: **2,4-Dioxopentanoic acid**, 9CI

Synonym(s): 2,4-Dioxovaleric acid, 8CI. Acetylpyruvic acid. Acetoneoxalic acid

CAS Registry Number: 5699-58-1

H3CCOCH2COCOOH

Molecular Formula: C5H6O4

Molecular Weight: 130.1

Accurate Mass: 130.02661

Percentage Composition: C 46.16%; H 4.65%; O 49.19%

Physical Description: Prisms (CCl₄)

Melting Point: Mp 98°

Boiling Point: Bp₃₇ 130°

Solubility: Sol. H₂O, EtOH, Et₂O, CHCl₃, C₆H₆

pKa Value: pK_{a1} 2.59; pK_{a2} 8.5 (25°)

Sigma: A6009

>>Derivative: Me ester

CAS Registry Number: 20577-61-1

Molecular Formula: C6H8O4

Molecular Weight: 144.127

Accurate Mass: 144.04226

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Use/Importance: Versatile photosynthon, giving [2+2] cycloadducts with alkenes *via* its enol form

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 63-64°

Boiling Point: Bp₁₂ 93-97°

Other Data: Enolises

>>Derivative: Et ester

CAS Registry Number: 615-79-2

Molecular Formula: C7H10O4

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Melting Point: Mp 16-18°

Boiling Point: Bp₃₇ 130°. Bp₁₂ 101-103°

Aldrich: 23256-4

Fluka: 730

>>Derivative: Amide

Molecular Formula: C5H7NO3

Molecular Weight: 129.115

Accurate Mass: 129.042594

Percentage Composition: C 46.51%; H 5.46%; N 10.85%; O 37.17%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 131-132 dec.°

Solubility: Sol. H₂O, Me₂CO, AcOH; insol. petrol

>>Derivative: Dioxime, Et ester

CAS Registry Number: 26074-63-5

Molecular Formula: C7H12N2O4

Molecular Weight: 188.183

Accurate Mass: 188.079708

Percentage Composition: C 44.68%; H 6.43%; N 14.89%; O 34.01%

Physical Description: Cryst. (EtOAc/C₆H₆)

Melting Point: Mp 128.5-130°

References: