



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

Synonym(s): Propionylpyruvic acid

CAS Registry Number: 4383-93-1

$\text{H}_3\text{CCH}_2\text{COCH}_2\text{COCOOH}$

Molecular Formula: $\text{C}_6\text{H}_8\text{O}_4$

Molecular Weight: 144.127

Accurate Mass: 144.04226

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

Physical Description: Cryst.

Melting Point: Mp 83°

>>Derivative: Me ester

CAS Registry Number: 20577-62-2

Molecular Formula: $\text{C}_7\text{H}_{10}\text{O}_4$

Molecular Weight: 158.154

Accurate Mass: 158.05791

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

Boiling Point: Bp₄ 90-95°

>>Derivative: Et ester

CAS Registry Number: 13246-52-1

Molecular Formula: $\text{C}_8\text{H}_{12}\text{O}_4$

Molecular Weight: 172.18

Accurate Mass: 172.07356

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

Boiling Point: Bp₁₁ 108-111°

References:

Breusch, F.L. *et al.*, *Enzymologia*, 1945, **11**, 356-360; *CA*, **40**, 5702, (*synth*)

Earl, E. *et al.*, *J.A.C.S.*, 1945, **67**, 1508-1509, (*Me ester*)

Schinz, H. *et al.*, *Helv. Chim. Acta*, 1947, **30**, 1349-1373, (*Et ester*)

Brecker, L. *et al.*, *New J. Chem.*, 1999, **23**, 437-446, (*synth, uv, pmr, cmr*)