



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

Synonym(s): 2,2-Dimethyllevulinic acid, 8CI. Mesitonic acid. Acetylpyvalic acid. 2,2-Dimethyl-4-oxovaleric acid

CAS Registry Number: 470-49-5

$\text{H}_3\text{CCOCH}_2\text{C}(\text{CH}_3)_2\text{COOH}$

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: Prisms (H_2O)

Melting Point: Mp 75.5-76.5°

Boiling Point: Bp₁₅ 138°

Solubility: Sol. H_2O , EtOH, Et₂O, C_6H_6

>>Derivative: Et ester

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}_3$

Molecular Weight: 172.224

Accurate Mass: 172.109945

Percentage Composition: C 62.77%; H 9.36%; O 27.87%

Boiling Point: Bp 210°

>>Derivative: Oxime

Molecular Formula: $\text{C}_7\text{H}_{13}\text{NO}_3$

Molecular Weight: 159.185

Accurate Mass: 159.089544

Percentage Composition: C 52.82%; H 8.23%; N 8.80%; O 30.15%

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 93-94°

Solubility: V. sol. H_2O , EtOH, Et₂O, sol. C_6H_6

>>Derivative: Phenylhydrazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 135°

>>Derivative: Semicarbazone

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 197.5 dec.°

References:

Lapworth, A., *J.C.S.*, 1904, **85**, 1218, (*synth*)

Pascual, C. *et al.*, *Helv. Chim. Acta*, 1964, **47**, 213, (*synth, ir, nmr*)