



>>Entry Name: **Methyloxobutanedioic acid**, 9CI

Synonym(s): Methyloxaloacetic acid, 8CI. 2-Oxalopropionic acid

CAS Registry Number: 642-93-3

HOOCCH(CH₃)COCOOH

Molecular Formula: C₅H₆O₅

Molecular Weight: 146.099

Accurate Mass: 146.021525

Percentage Composition: C 41.11%; H 4.14%; O 54.76%

>>Variant: (±)-form

Molecular Formula: C₅H₆O₅

Molecular Weight: 146.099

Accurate Mass: 146.021525

Percentage Composition: C 41.11%; H 4.14%; O 54.76%

Melting Point: Mp 142-143°

>>Derivative: Di-Et ester

CAS Registry Number: 759-65-9

Molecular Formula: C₉H₁₄O₅

Molecular Weight: 202.207

Accurate Mass: 202.084125

Percentage Composition: C 53.46%; H 6.98%; O 39.56%

Physical Description: Liq.

Boiling Point: Bp₂₃ 137-138°. Bp₁₀ 114-116°

Solubility: Misc. EtOH, Et₂O; insol. H₂O

pKa Value: pK_{a1} 7.03

Other Data: Dec. on standing

Fluka: 75680

>>Derivative: Phenylhydrazone

Melting Point: Mp 99-100°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 164°. Mp 188-189° (double Mp)

>>Derivative: Mononitrile

Molecular Formula: C₅H₅NO₃

Molecular Weight: 127.099

Accurate Mass: 127.026944

Percentage Composition: C 47.25%; H 3.97%; N 11.02%; O 37.76%

Physical Description: Yellow cryst. (Et₂O/petrol)

Melting Point: Mp 207-208°

Solubility: Sol. H₂O, insol. C₆H₆

References:

Wislicenus, W. *et al.*, *Annalen*, 1888, **246**, 329, (*deriv*)

Wislicenus, W. *et al.*, *Ber.*, 1910, **43**, 1829, (*deriv*)

Gulegov, G.A., *Biokhimiya (Moscow)*, 1961, **26**, 560, (*synth*)

Sakkeb, N.Y. *et al.*, *J.A.C.S.*, 1976, **98**, 5285, (*nmr*)