



>>Entry Name: 2-Acetyl-3-oxobutanoic acid, 9CI

Synonym(s): 2-Acetylacetoacetic acid. Diacetylacetic acid

CAS Registry Number: 4433-82-3

(CH₃CO)₂CHCOOH

Molecular Formula: C₆H₈O₄

Molecular Weight: 144.127

Accurate Mass: 144.04226

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

>>Derivative: Me ester

CAS Registry Number: 4619-66-3

Molecular Formula: C₇H₁₀O₄

Molecular Weight: 158.154

Accurate Mass: 158.05791

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

Boiling Point: Bp_{0.5} 48-50°

Fluka: 890

>>Derivative: Et ester

CAS Registry Number: 603-69-0

Molecular Formula: C₈H₁₂O₄

Molecular Weight: 172.18

Accurate Mass: 172.07356

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

Boiling Point: Bp₁₆ 104°

>>Derivative: Nitrile

Synonym(s): 2-Acetyl-3-oxobutanenitrile, 9CI. 3-Cyano-2,4-pentanedione

CAS Registry Number: 3141-59-1

Molecular Formula: C₆H₇NO₂

Molecular Weight: 125.127

Accurate Mass: 125.047679

Percentage Composition: C 57.59%; H 5.64%; N 11.19%; O 25.57%

Physical Description: Leaflets

Melting Point: Mp 50°

References:

Claisen, L. *et al.*, *Annalen*, 1893, **277**, 162, (*synth*)

Packendorff, K., *Ber.*, 1931, **64**, 948, (*synth*)

Org. Synth., *Coll. Vol.*, 3, 1955, 390, (*synth*)

Martin, D. *et al.*, *Chem. Ber.*, 1965, **98**, 3662, (*synth*)

Harries, H.J. *et al.*, *Inorg. Chim. Acta*, 1978, **31**, 233, (*ms*)

Niclas, H.-J. *et al.*, *Synth. Commun.*, 1994, **24**, 3241, (*nitrile*)

Bohář, A. *et al.*, *Synthesis*, 1994, 381, (*synth, pmr*)

Brassard, P. *et al.*, *Synthesis*, 1994, 703, (*Me ester*)