



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

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

CAS Registry Number: 4433-82-3

$(\text{CH}_3\text{CO})_2\text{CHCOOH}$

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%

>>Derivative: Me ester

CAS Registry Number: 4619-66-3

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: $\text{Bp}_{0.5}$ 48-50°

Fluka: 890

>>Derivative: Et ester

CAS Registry Number: 603-69-0

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: Bp_{16} 104°

>>Derivative: Nitrile

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

CAS Registry Number: 3141-59-1

Molecular Formula: $\text{C}_6\text{H}_7\text{NO}_2$

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: