



Boiling Point: Bp_{0.13} 76°

Fluka: 470

Rare Chemicals Library: S40762-3

>> **Derivative:** Nitrile

Synonym(s): 3-Oxobutanenitrile, 9CI. Cyanoacetone. Acetoacetonitrile

CAS Registry Number: 2469-99-0

Molecular Formula: C₄H₅NO

Molecular Weight: 83.09

Accurate Mass: 83.037114

Percentage Composition: C 57.82%; H 6.07%; N 16.86%; O 19.26%

Physical Description: Liq.

Boiling Point: Bp 230° dec.

Other Data: Polymerises

>> **Derivative:** 2-Methylpropyl ester

Synonym(s): 2-Methylpropyl 3-oxobutanoate. Isobutyl acetoacetate. FEMA 1277

CAS Registry Number: 7779-75-1

Molecular Formula: C₈H₁₄O₃

Molecular Weight: 158.197

Accurate Mass: 158.094295

Percentage Composition: C 60.74%; H 8.92%; O 30.34%

Use/Importance: Flavouring ingredient

Physical Description: Liq.

Boiling Point: Bp₁₁ 84.5°

Density: d²⁵ 0.97

Refractive Index: n_D²⁵ 1.4219

>> **Derivative:** 3-Methylbutyl ester

Synonym(s): 3-Methylbutyl 3-oxobutanoate. Isoamyl acetoacetate. FEMA 3551

CAS Registry Number: 2308-18-1

Molecular Formula: C₉H₁₆O₃

Molecular Weight: 172.224

Accurate Mass: 172.109945

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

Use/Importance: Flavouring ingredient

Boiling Point: Bp 222-224°

>> **Variant:** Oxo-form

Molecular Formula: C₄H₆O₃

Molecular Weight: 102.09

Accurate Mass: 102.031695

Percentage Composition: C 47.06%; H 5.92%; O 47.02%

>> **Derivative:** Phenylhydrazone

Molecular Formula: C₁₀H₁₂N₂O₂

Molecular Weight: 192.217

Accurate Mass: 192.089878

Percentage Composition: C 62.49%; H 6.29%; N 14.57%; O 16.65%

Melting Point: Mp 128°

>> **Variant:** Enol-form

Synonym(s): 3-Hydroxy-2-butenic acid. 3-Hydroxycrotonic acid

Molecular Formula: C₄H₆O₃

Molecular Weight: 102.09

Accurate Mass: 102.031695

Percentage Composition: C 47.06%; H 5.92%; O 47.02%