



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

Synonym(s): 2-Methylacetoacetic acid, 8CI. 2-Acetylpropanoic acid

CAS Registry Number: 2382-59-4

H3CCOCH(CH3)COOH

Molecular Formula: C5H8O3

Molecular Weight: 116.116

Accurate Mass: 116.047345

Percentage Composition: C 51.72%; H 6.94%; O 41.34%

>>Variant: (±)-form

Molecular Formula: C5H8O3

Molecular Weight: 116.116

Accurate Mass: 116.047345

Percentage Composition: C 51.72%; H 6.94%; O 41.34%

Physical Description: Oil

Boiling Point: Bp₃₄ 224°

Solubility: Sol. H₂O

>>Derivative: Me ester

CAS Registry Number: 609-14-3

Extra CAS Registry Numbers(s): 17094-21-2

Molecular Formula: C6H10O3

Molecular Weight: 130.143

Accurate Mass: 130.062995

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

Boiling Point: Bp 177.4°. Bp₂₀ 80°

Refractive Index: n_D²¹ 1.4183

Aldrich: E3540-0

>>Derivative: Amide

CAS Registry Number: 4433-76-5

Molecular Formula: C5H9NO2

Molecular Weight: 115.132

Accurate Mass: 115.063329

Percentage Composition: C 52.16%; H 7.88%; N 12.17%; O 27.79%

Physical Description: Needles (Et₂O)

Melting Point: Mp 72-73°

>>Derivative: Nitrile

Synonym(s): 3-Cyano-2-butanone

CAS Registry Number: 4468-47-7

Molecular Formula: C5H7NO

Molecular Weight: 97.116

Accurate Mass: 97.052764

Percentage Composition: C 61.84%; H 7.26%; N 14.42%; O 16.47%

Boiling Point: Bp 145-146°. Bp₁₉ 78°

Solubility: Misc. EtOH, Et₂O, C₆H₆, CHCl₃

>>Derivative: Nitrile, semicarbazone

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 153°

References: