



>>Entry Name: 2-Oxobutanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3-Methylpyruvic acid. 2-Ketobutyric acid. FEMA 3723

CAS Registry Number: 600-18-0

$\text{H}_3\text{CCH}_2\text{COCOOH}$

Molecular Formula: $\text{C}_4\text{H}_6\text{O}_3$

Molecular Weight: 102.09

Accurate Mass: 102.031695

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

Biological Source: Prod. by *Saccharomyces cerevisiae*, *Ceratocystis variispora* and other microorganisms

Physical Description: Plates

Melting Point: Mp 31-32°

Boiling Point: Bp₁₂ 66°

Solubility: Sol. H₂O, ETOH

pKa Value: pK_{a1} 2.5 (25°)

Aldrich: W37230-7

Fluka: 75820

Sigma: K8875

>>Derivative: Oxime

Synonym(s): 2-(Hydroxyimino)butanoic acid, 9CI

CAS Registry Number: 609-30-3

Molecular Formula: $\text{C}_4\text{H}_7\text{NO}_3$

Molecular Weight: 117.104

Accurate Mass: 117.042594

Percentage Composition: C 41.03%; H 6.02%; N 11.96%; O 40.99%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 167°

>>Derivative: Phenylhydrazone

Physical Description: Cryst. (C₆H₆/EtOH)

Melting Point: Mp 210°

>>Derivative: Semicarbazone

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 210°

>>Derivative: Me ester

CAS Registry Number: 3952-66-7

Molecular Formula: $\text{C}_5\text{H}_8\text{O}_3$

Molecular Weight: 116.116

Accurate Mass: 116.047345

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

Physical Description: Liq.

Boiling Point: Bp₂₇ 72-74°

>>Derivative: Et ester

CAS Registry Number: 15933-07-0

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_3$

Molecular Weight: 130.143

Accurate Mass: 130.062995

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

Physical Description: Liq.

Boiling Point: Bp 162°. Bp₁₆ 66°

Aldrich: 16410-0