



>>Entry Name: 3-Methyl-2-oxobutanoic acid

ENTRY UNDER REVIEW

Synonym(s): 2-Oxoisopentanoic acid. α -Ketoisovaleric acid. Dimethylpyruvic acid

CAS Registry Number: 759-05-7

$(\text{H}_3\text{C})_2\text{CHCOCOOH}$

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%

Biological Source: Metab. of *Aspergillus niger* and other microorganisms

Use/Importance: Inhibits pyruvate transport in rat liver mitochondria

Physical Description: Cryst.

Melting Point: Mp 31°

Boiling Point: Bp 170.5°

>>Derivative: Na salt

CAS Registry Number: 3715-29-5

Melting Point: Mp 227-230°

Aldrich: 19899-4

Fluka: 68253

Sigma: K4875

>>Derivative: Oxime

CAS Registry Number: 13010-50-9

Molecular Formula: $\text{C}_5\text{H}_9\text{NO}_3$

Molecular Weight: 131.131

Accurate Mass: 131.058244

Percentage Composition: C 45.80%; H 6.92%; N 10.68%; O 36.60%

Physical Description: Cryst.

Melting Point: Mp 163-165 dec.°

>>Derivative: Phenylhydrazone

Physical Description: Long yellow needles (MeOH aq.)

Melting Point: Mp 156-157°

>>Derivative: Me ester

CAS Registry Number: 3952-67-8

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%

Boiling Point: Bp₁₂ 70-80°

>>Derivative: Me ester, 2,4-dinitrophenylhydrazone

Physical Description: Cryst.

Melting Point: Mp 176-178°

>>Derivative: Et ester

CAS Registry Number: 20201-24-5

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_3$

Molecular Weight: 144.17

Accurate Mass: 144.078645

Percentage Composition: C 58.32%; H 8.39%; O 33.29%

Boiling Point: Bp₁₀ 58-60°

Aldrich: 21845-6

Fluka: 68251

>>Derivative: Et ester, oxime