



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

Synonym(s): 2-Oxocaproic acid

CAS Registry Number: 2492-75-3

$\text{H}_3\text{C}(\text{CH}_2)_3\text{COCO}_2\text{H}$

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%

Biological Source: Isol. from cultures of *Ceratocystis variispora*

Physical Description: Cryst.

Melting Point: Mp 15°

Boiling Point: Bp₆ 78°

>>Derivative: Na salt

CAS Registry Number: 13022-85-0

Physical Description: Solid

Melting Point: Mp 235 dec.°

Aldrich: 28637-0

Sigma: K6625

>>Derivative: Oxime

CAS Registry Number: 21486-55-5

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}_3$

Molecular Weight: 145.158

Accurate Mass: 145.073894

Percentage Composition: C 49.65%; H 7.64%; N 9.65%; O 33.07%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 140°

>>Derivative: Semicarbazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 180°

>>Derivative: Et ester

CAS Registry Number: 5753-96-8

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_3$

Molecular Weight: 158.197

Accurate Mass: 158.094295

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

Boiling Point: Bp₁₀ 84°

>>Derivative: Et ester, semicarbazone

Physical Description: Prisms (MeOH)

Melting Point: Mp 149°

References:

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Schreiber, J., *Bull. Soc. Chim. Fr.*, 1956, 1361, (synth)

Lapkin, I.I. *et al.*, *CA*, 1962, **57**, 11010, (synth)

Jain, S. *et al.*, *Acta Cryst.*, 1966, **21**, 455, (cryst struct)

Collins, R.P. *et al.*, *J. Nat. Prod.*, 1966, **29**, 245, (isol)

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Ramage, R. *et al.*, *J.C.S. Perkin 1*, 1984, 1531, (synth, ir)