



>>Entry Name: 5-Oxohexanoic acid, 9CI

Synonym(s): 4-Acetylbutyric acid. 5-Oxocaproic acid

CAS Registry Number: 3128-06-1

H3CCOCH2CH2CH2COOH

Molecular Formula: C6H10O3

Molecular Weight: 130.143

Accurate Mass: 130.062995

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

Melting Point: Mp 13-14°

Boiling Point: Bp 275° sl. dec.. Bp_{2.5} 130-131°

Refractive Index: n_D²⁰ 1.4462

Aldrich: A1320-4

Sigma: A3896

>>Derivative: Oxime

Molecular Formula: C6H11NO3

Molecular Weight: 145.158

Accurate Mass: 145.073894

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

Physical Description: Prisms (C6H6)

Melting Point: Mp 104-105°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 143°

>>Derivative: Me ester

CAS Registry Number: 13984-50-4

Molecular Formula: C7H12O3

Molecular Weight: 144.17

Accurate Mass: 144.078645

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

Boiling Point: Bp₈ 90-91°

Rare Chemicals Library: S86098-0

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

CAS Registry Number: 13984-51-5

Physical Description: Golden plates (MeOH)

Melting Point: Mp 88-89°

>>Derivative: Et ester

CAS Registry Number: 13984-57-1

Molecular Formula: C8H14O3

Molecular Weight: 158.197

Accurate Mass: 158.094295

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

Boiling Point: Bp 222°. Bp₃ 83-84°

Aldrich: 19209-0

>>Derivative: Et ester, semicarbazone

Melting Point: Mp 115°