



>>Entry Name: 3-Oxopentanoic acid, 9Cl

Synonym(s): Propionylacetic acid

CAS Registry Number: 10191-25-0

H3CCH2COCH2COOH

Molecular Formula: C5H8O3

Molecular Weight: 116.116

Accurate Mass: 116.047345

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

Physical Description: Needles (Et₂O/hexane)

Melting Point: Mp 65-66 dec.°

>>Derivative: Cu deriv.

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 160-161°

>>Derivative: Me ester

CAS Registry Number: 30414-53-0

Molecular Formula: C6H10O3

Molecular Weight: 130.143

Accurate Mass: 130.062995

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

Physical Description: Oil

Boiling Point: Bp₁₆ 73-76°

Aldrich: 25587-4

Fluka: 75957

Rare Chemicals Library: S12965-8

>>Derivative: Et ester

CAS Registry Number: 4949-44-4

Molecular Formula: C7H12O3

Molecular Weight: 144.17

Accurate Mass: 144.078645

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

Physical Description: Oil

Boiling Point: Bp 191°. Bp₉ 83-86°

pKa Value: pK_{a1} 11.07 (26°)

Aldrich: 24716-2

Fluka: 75953

>>Derivative: *tert*-Butyl ester

Synonym(s): *tert*-Butyl propionylacetate

CAS Registry Number: 33400-61-2

Molecular Formula: C9H16O3

Molecular Weight: 172.224

Accurate Mass: 172.109945

Percentage Composition: C 62.77%; H 9.36%; O 27.87%

Physical Description: Oil

Boiling Point: Bp_{0.2} 49.5-50.5°

>>Derivative: Benzyl ester

Synonym(s): Benzyl propionylacetate

CAS Registry Number: 4949-45-5

Molecular Formula: C12H14O3

Molecular Weight: 206.241

Accurate Mass: 206.094295

Percentage Composition: C 69.89%; H 6.84%; O 23.27%

Physical Description: Oil

Boiling Point: Bp_{0.16} 93-103°