



>>Entry Name: 2-Ethyl-3-oxobutanoic acid, 9CI

Synonym(s): 2-Acetylbutyric acid

CAS Registry Number: 4433-85-6

H3CCOCH(COOH)CH2CH3

Molecular Formula: C6H10O3

Molecular Weight: 130.143

Accurate Mass: 130.062995

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

>>Variant: (±)-form

Molecular Formula: C6H10O3

Molecular Weight: 130.143

Accurate Mass: 130.062995

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

>>Derivative: Me ester

CAS Registry Number: 51756-08-2

Molecular Formula: C7H12O3

Molecular Weight: 144.17

Accurate Mass: 144.078645

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

Boiling Point: Bp 190°

>>Derivative: Et ester

CAS Registry Number: 607-97-6

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 198°. Bp₇ 70-71°

Solubility: Mod. sol. H₂O

Density: d₄²⁵ 0.975

pKa Value: pK_{a1} 13 (23°)

Refractive Index: n_D¹⁹ 1.4226

Aldrich: 16526-3

Fluka: 2840

Sigma: A6305

>>Derivative: Et ester, semicarbazone

Physical Description: Cryst.

Melting Point: Mp 154 dec.°

>>Derivative: Amide

Molecular Formula: C6H11NO2

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Physical Description: Needles (H₂O)

Boiling Point: Subl. 95-96°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1096C, (nmr)

Michael, A., *J. Prakt. Chem.*, 1905, **72**, 553

Ioffe, S.T. *et al.*, *Tet. Lett.*, 1965, 593

Jacquier, R. *et al.*, *Bull. Soc. Chim. Fr.*, 1969, 3694