



>>Entry Name: Acetylbutanedioic acid

Synonym(s): Acetylsuccinic acid. 3-Carboxy-4-oxopentanoic acid

Related CAS Registry Numbers(s): 10420-33-4

$\text{H}_3\text{CCOCH}(\text{COOH})\text{CH}_2\text{COOH}$

Molecular Formula: $\text{C}_6\text{H}_8\text{O}_5$

Molecular Weight: 160.126

Accurate Mass: 160.037175

Percentage Composition: C 45.01%; H 5.04%; O 49.96%

>>Variant: ($\pm$)-form

Molecular Formula: $\text{C}_6\text{H}_8\text{O}_5$

Molecular Weight: 160.126

Accurate Mass: 160.037175

Percentage Composition: C 45.01%; H 5.04%; O 49.96%

pKa Value: $\text{p}K_{\text{a}1}$ 2.86; $\text{p}K_{\text{a}2}$ 4.57 (25°)

>>Derivative: Di-Me ester

Synonym(s): Dimethyl acetylsuccinate, 8CI

CAS Registry Number: 121952-83-8

Molecular Formula: $\text{C}_8\text{H}_{12}\text{O}_5$

Molecular Weight: 188.18

Accurate Mass: 188.068475

Percentage Composition: C 51.06%; H 6.43%; O 42.51%

Melting Point: Mp 33°

Boiling Point: Bp_{12} 129-134°

>>Derivative: Di-Me ester, phenylhydrazone

Physical Description: Cryst.

Melting Point: Mp 198-201°

>>Derivative: Di-Et ester

CAS Registry Number: 1115-30-6

Physical Description: Liq.

Boiling Point: Bp 254-256° (dec.). Bp_{15} 140-142°

Aldrich: D8540-3

>>Derivative: Di-Et ester, phenylhydrazone

Physical Description: Cryst.

Melting Point: Mp 155-157°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 691D, (*ir*)

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1110B, (*nmr*)

Fittig, R. *et al.*, *Annalen*, 1894, **283**, 67, (*synth, deriv*)

Org. Synth., *Coll. Vol.*, 2, 1943, 262, (*synth*)

Patrick, T.M., *J.O.C.*, 1952, **17**, 1009, (*di-Me ester*)

Nagasaka, A. *et al.*, *Bull. Inst. Chem. Res., Kyoto Univ.*, 1954, **32**, 238, (*di-Me ester*)

Stille, J.K. *et al.*, *J.O.C.*, 1979, **44**, 3474, (*synth, ir, pmr, di-Me ester*)

Craig, G.W. *et al.*, *J. Prakt. Chem.*, 2000, **342**, 504-507, (*di-Me ester, use*)