



>>Entry Name: Di-2-propenylpropanedioic acid, 9CI

Synonym(s): Diallylmalonic acid. 1,6-Heptadiene-4,4-dicarboxylic acid

CAS Registry Number: 4372-31-0

$(\text{H}_2\text{C}=\text{CHCH}_2)_2\text{C}(\text{COOH})_2$

Molecular Formula: $\text{C}_9\text{H}_{12}\text{O}_4$

Molecular Weight: 184.191

Accurate Mass: 184.07356

Percentage Composition: C 58.69%; H 6.57%; O 34.75%

Physical Description: Cryst. (H_2O or C_6H_6)

Melting Point: Mp 135-137°

pKa Value: $\text{p}K_{\text{a}}$ 2.1 (25°)

>>Derivative: Di-Et ester

CAS Registry Number: 3195-24-2

Molecular Formula: $\text{C}_{13}\text{H}_{20}\text{O}_4$

Molecular Weight: 240.299

Accurate Mass: 240.13616

Percentage Composition: C 64.98%; H 8.39%; O 26.63%

Boiling Point: Bp_{12} 120-122°

Aldrich: 28347-9

Rare Chemicals Library: S52132-9

>>Derivative: Diamide

Molecular Formula: $\text{C}_9\text{H}_{14}\text{N}_2\text{O}_2$

Molecular Weight: 182.222

Accurate Mass: 182.105528

Percentage Composition: C 59.32%; H 7.74%; N 15.37%; O 17.56%

Melting Point: Mp 202°

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 996C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 640A, (*ir*)

Leuchs, H. *et al.*, *Ber.*, 1914, **47**, 2573, (*synth*)

Shimo, K. *et al.*, *J.O.C.*, 1959, **24**, 19, (*synth*)