



>>Entry Name: 2-Propenylpropanedioic acid, 9CI

Synonym(s): Allylmalonic acid. 1-Butene-4,4-dicarboxylic acid

CAS Registry Number: 2583-25-7

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

Molecular Formula: $\text{C}_6\text{H}_8\text{O}_4$

Molecular Weight: 144.127

Accurate Mass: 144.04226

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Physical Description: Cryst. (Et_2O)

Melting Point: Mp 105°

Solubility: Sol. H_2O , Et_2O , EtOH , hot C_6H_6

pKa Value: $\text{p}K_{\text{a}}$ 2.8

Fluka: 6023

>>Derivative: Ag salt

Melting Point: Mp 60 dec.°

Solubility: Insol. H_2O

>>Derivative: Di-Et ester

CAS Registry Number: 2049-80-1

Molecular Formula: $\text{C}_{10}\text{H}_{16}\text{O}_4$

Molecular Weight: 200.234

Accurate Mass: 200.10486

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Boiling Point: Bp $222\text{--}223^\circ$. Bp₆ 93°

Aldrich: 44611-4

Fluka: 6022

Sigma: D8635

>>Derivative: Amide

Molecular Formula: $\text{C}_6\text{H}_9\text{NO}_3$

Molecular Weight: 143.142

Accurate Mass: 143.058244

Percentage Composition: C 50.35%; H 6.34%; N 9.79%; O 33.53%

Melting Point: Mp 98°

Boiling Point: Bp 289°

References:

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

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 646D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 692C, (*ir*)

Conrad, M., *Annalen*, 1880, **204**, 168, (*synth*)