



>>Entry Name: Propylpropanedioic acid

Synonym(s): Propylmalonic acid. Butane-1,1-dicarboxylic acid

CAS Registry Number: 616-62-6

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

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_4$

Molecular Weight: 146.143

Accurate Mass: 146.05791

Percentage Composition: C 49.31%; H 6.90%; O 43.79%

Physical Description: Plates (C_6H_6)

Melting Point: Mp 96°

Solubility: V. sol. H_2O

pKa Value: $\text{p}K_{\text{a}1}$ 3; $\text{p}K_{\text{a}2}$ 5.84 (25°)

>>Derivative: Di-Me ester

CAS Registry Number: 14035-96-2

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_4$

Molecular Weight: 174.196

Accurate Mass: 174.08921

Percentage Composition: C 55.16%; H 8.10%; O 36.74%

Physical Description: Liq.

>>Derivative: Di-Et ester

CAS Registry Number: 2163-48-6

Molecular Formula: $\text{C}_{10}\text{H}_{18}\text{O}_4$

Molecular Weight: 202.25

Accurate Mass: 202.12051

Percentage Composition: C 59.39%; H 8.97%; O 31.64%

Boiling Point: Bp 235°. Bp₄₀ 145°

Aldrich: 22881-8

Fluka: 82365

Sigma: D2136

>>Derivative: Di-Ph ester

Molecular Formula: $\text{C}_{18}\text{H}_{18}\text{O}_4$

Molecular Weight: 298.338

Accurate Mass: 298.12051

Percentage Composition: C 72.47%; H 6.08%; O 21.45%

Physical Description: Liq.

Boiling Point: Bp₁₈ 213°

>>Derivative: Diamide

Molecular Formula: $\text{C}_6\text{H}_{12}\text{N}_2\text{O}_2$

Molecular Weight: 144.173

Accurate Mass: 144.089878

Percentage Composition: C 49.99%; H 8.39%; N 19.43%; O 22.19%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 184°

>>Derivative: Dianilide

Molecular Formula: $\text{C}_{18}\text{H}_{20}\text{N}_2\text{O}_2$

Molecular Weight: 296.368

Accurate Mass: 296.152478

Percentage Composition: C 72.95%; H 6.80%; N 9.45%; O 10.80%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 198°