



>>Entry Name: Isopropylpropanedioic acid

Synonym(s): Isopropylmalonic acid, 8Cl. Isobutane-1,1-dicarboxylic acid. 2-Methylpropane-1,1-dicarboxylic acid

CAS Registry Number: 601-79-6

$(\text{H}_3\text{C})_2\text{CHCH}(\text{COOH})_2$

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%

Use/Importance: Monosubstd. derivs. used as chiral reagents

Melting Point: Mp 87°

pKa Value: $\text{p}K_{\text{a}1}$ 2.92; $\text{p}K_{\text{a}2}$ 5.88 (25°, H_2O) $\text{p}K_{\text{a}1}$ 2.92; $\text{p}K_{\text{a}2}$ 3.43

Other Data: Dec. at 108°

Rare Chemicals Library: S56744-2

>>Derivative: Mono-Me ester

>>Derivative: Di-Me ester

CAS Registry Number: 51122-91-9

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%

Boiling Point: Bp_{770} 195°

>>Derivative: Di-Et ester

CAS Registry Number: 759-36-4

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_{748} 215-217°

>>Derivative: Monoamide

References:

Volwiler, E.H. *et al.*, *J.A.C.S.*, 1930, **52**, 1676, (*esters*)

Marshall, F.C.B., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1932, **51**, 236, (*synth*)

Hayashi, T. *et al.*, *J.A.C.S.*, 1977, **99**, 7093, (*ester*)