



>>Entry Name: Benzylpropanedioic acid

Synonym(s): (Phenylmethyl)propanedioic acid, 9CI. Benzylmalonic acid, 8CI

CAS Registry Number: 616-75-1

Related CAS Registry Numbers(s): 42361-66-0 67682-05-7 82527-49-9 114746-79-1

$\text{PhCH}_2\text{CH}(\text{COOH})_2$

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

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Physical Description: Cryst. (Et_2O)

Melting Point: Mp 121° (117°)

Solubility: Sol. hot H_2O

pKa Value: $\text{p}K_{\text{a}1}$ 2.91; $\text{p}K_{\text{a}2}$ 5.87 (25°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 200 mg/kg

Aldrich: 10077-3

Fluka: 13530

>>Derivative: Di-Me ester

CAS Registry Number: 49769-78-0

Molecular Formula: $\text{C}_{12}\text{H}_{14}\text{O}_4$

Molecular Weight: 222.24

Accurate Mass: 222.08921

Percentage Composition: C 64.85%; H 6.35%; O 28.80%

Physical Description: Oil

Boiling Point: Bp 282-285°

>>Derivative: Mono-Et ester

CAS Registry Number: 2985-39-9

Molecular Formula: $\text{C}_{12}\text{H}_{14}\text{O}_4$

Molecular Weight: 222.24

Accurate Mass: 222.08921

Percentage Composition: C 64.85%; H 6.35%; O 28.80%

Physical Description: Oil

Refractive Index: n_{D}^{19} 1.5107

>>Derivative: Di-Et ester

CAS Registry Number: 607-81-8

Molecular Formula: $\text{C}_{14}\text{H}_{18}\text{O}_4$

Molecular Weight: 250.294

Accurate Mass: 250.12051

Percentage Composition: C 67.18%; H 7.25%; O 25.57%

Physical Description: Oil

Boiling Point: Bp 300°. Bp₁₂ 169°

Density: d_{15}^{15} 1.077

Aldrich: 13554-2

Fluka: 13532

Sigma: B3777

>>Derivative: Di-tert-butyl ester

CAS Registry Number: 41890-49-7

Molecular Formula: $\text{C}_{18}\text{H}_{26}\text{O}_4$

Molecular Weight: 306.401

Accurate Mass: 306.18311

Percentage Composition: C 70.56%; H 8.55%; O 20.89%

Physical Description: Oil

Boiling Point: Bp_{0.9} 115-117°

Refractive Index: n_{D}^{25} 1.4682