



>>Entry Name: Benzylidenepropanedioic acid

Synonym(s): Phenylmethylenepropanedioic acid, 9CI. Benzylidenemalonic acid. Benzalmalonic acid

CAS Registry Number: 584-45-2

$\text{PhCH}=\text{C}(\text{COOH})_2$

Molecular Formula: $\text{C}_{10}\text{H}_8\text{O}_4$

Molecular Weight: 192.171

Accurate Mass: 192.04226

Percentage Composition: C 62.50%; H 4.20%; O 33.30%

Physical Description: Prisms (EtOH)

Melting Point: Mp 195-196 dec.°

pKa Value: $\text{p}K_{\text{a}1}$ 2.39; $\text{p}K_{\text{a}2}$ 5.5 (25°, H_2O) $\text{p}K_{\text{a}1}$ 4; $\text{p}K_{\text{a}2}$ 6.7 (25°)

Rare Chemicals Library: S8060-9

>>Derivative: Di-Me ester

CAS Registry Number: 6626-84-2

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

Molecular Weight: 220.224

Accurate Mass: 220.07356

Percentage Composition: C 65.45%; H 5.49%; O 29.06%

Melting Point: Mp 45°

Boiling Point: Bp_{10} 171°

Rare Chemicals Library: S54548-1

>>Derivative: Mono-Et ester

CAS Registry Number: 110882-40-1

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

Molecular Weight: 220.224

Accurate Mass: 220.07356

Percentage Composition: C 65.45%; H 5.49%; O 29.06%

Melting Point: Mp 85°

>>Derivative: Di-Et ester

CAS Registry Number: 5292-53-5

Molecular Formula: $\text{C}_{14}\text{H}_{16}\text{O}_4$

Molecular Weight: 248.278

Accurate Mass: 248.10486

Percentage Composition: C 67.73%; H 6.50%; O 25.78%

Melting Point: Mp 32°

Boiling Point: Bp_{14} 196°. Bp_5 176-177°

Density: d_4^{20} 1.1

Aldrich: D9020-2

Fluka: 13471

Rare Chemicals Library: S3608-1

Sigma: D8385

>>Derivative: Dichloride

CAS Registry Number: 32046-40-5

Molecular Formula: $\text{C}_{10}\text{H}_6\text{Cl}_2\text{O}_2$

Molecular Weight: 229.062

Accurate Mass: 227.974484

Percentage Composition: C 52.44%; H 2.64%; Cl 30.95%; O 13.97%

Physical Description: Needles (petrol)

Melting Point: Mp 77°

>>Derivative: Mononitrile

see 2-Cyano-3-phenyl-2-propenoic acid, [CXS90-L](#)