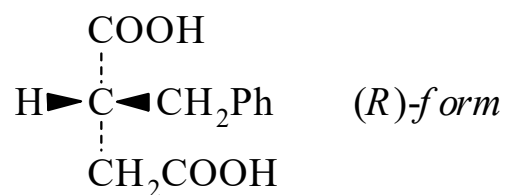




>>Entry Name: Benzylbutanedioic acid

Synonym(s): (Phenylmethyl)butanedioic acid, 9CI. Benzylsuccinic acid, 8CI



CAS Registry Number: 884-33-3

Related CAS Registry Numbers(s): 21307-94-8 79909-18-5

Molecular Formula: $\text{C}_{11}\text{H}_{12}\text{O}_4$

Molecular Weight: 208.213

Accurate Mass: 208.07356

Percentage Composition: C 63.45%; H 5.81%; O 30.74%

Rare Chemicals Library: S84605-8

>>Variant: (R)-form

CAS Registry Number: 21307-97-1

Molecular Formula: $\text{C}_{11}\text{H}_{12}\text{O}_4$

Molecular Weight: 208.213

Accurate Mass: 208.07356

Percentage Composition: C 63.45%; H 5.81%; O 30.74%

Melting Point: Mp 162-163°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +27$ (EtOAc)

>>Derivative: Di-Et ester

Molecular Formula: $\text{C}_{15}\text{H}_{20}\text{O}_4$

Molecular Weight: 264.321

Accurate Mass: 264.13616

Percentage Composition: C 68.16%; H 7.63%; O 24.21%

Physical Description: Oil

Boiling Point: Bp₅ 169-171°

Optical Rotation: $[\alpha]_{\text{D}}^{27.5} \mp 17.6$ (EtOH)

>>Derivative: 4-tert-Butyl ester

CAS Registry Number: 122225-33-6

Molecular Formula: $\text{C}_{15}\text{H}_{20}\text{O}_4$

Molecular Weight: 264.321

Accurate Mass: 264.13616

Percentage Composition: C 68.16%; H 7.63%; O 24.21%

Physical Description: Cryst.

Melting Point: Mp 56-58°

Optical Rotation: $[\alpha]_{\text{D}} +6.4$ (c, 0.11 in CHCl_3)

>>Derivative: 1-Benzyl ester

CAS Registry Number: 116129-80-7

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: Oil, cryst. on standing

Optical Rotation: $[\alpha]_{\text{D}}^{25} +11.3$ (c, 1 in MeOH)

>>Variant: (S)-form

CAS Registry Number: 3972-36-9

Molecular Formula: $\text{C}_{11}\text{H}_{12}\text{O}_4$

Molecular Weight: 208.213

Accurate Mass: 208.07356

Percentage Composition: C 63.45%; H 5.81%; O 30.74%

Melting Point: Mp 159-161°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -27$ (EtOAc)