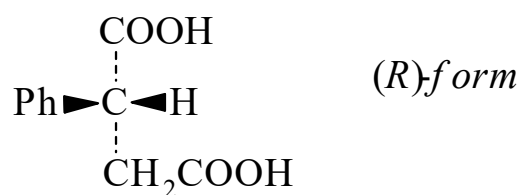




>>Entry Name: Phenylbutanedioic acid, 9CI

Synonym(s): Phenylsuccinic acid, 8CI



CAS Registry Number: 635-51-8

Related CAS Registry Numbers(s): 1131-15-3 112489-85-7

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

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

Aldrich: P3520-0

Fluka: 78170

>>Variant: (*R*)-form

CAS Registry Number: 46292-93-7

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

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

Melting Point: Mp 173-174°

Optical Rotation: $[\alpha]_{\text{D}}^{14} -173.3$ (Me₂CO)

Fluka: 78172

>>Derivative: Anhydride

CAS Registry Number: 116668-57-6

Molecular Formula: C₁₀H₈O₃

Molecular Weight: 176.171

Accurate Mass: 176.047345

Percentage Composition: C 68.18%; H 4.58%; O 27.25%

Melting Point: Mp 83.5-84.5°

Optical Rotation: $[\alpha]_{\text{D}}^{14} -100.9$ (C₆H₆)

>>Variant: (*S*)-form

CAS Registry Number: 4036-30-0

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

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

Physical Description: Prisms (H₂O)

Melting Point: Mp 173-174°

Optical Rotation: $[\alpha]_{\text{D}}^{15} +173.4$ (Me₂CO)

Fluka: 78173

>>Derivative: Di-Me ester

CAS Registry Number: 61548-76-3

Molecular Formula: C₁₂H₁₄O₄

Molecular Weight: 222.24

Accurate Mass: 222.08921

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

Boiling Point: Bp₁₆ 161-162°. Bp₂ 119°

Other Data: Racemised by MeONa in MeOH