



>>Entry Name: 3-Phenylpentanedioic acid, 9CI

Synonym(s): 3-Phenylglutaric acid

CAS Registry Number: 4165-96-2

PhCH(CH₂COOH)₂

Molecular Formula: C₁₁H₁₂O₄

Molecular Weight: 208.213

Accurate Mass: 208.07356

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

Physical Description: Plates (H₂O), prisms (C₆H₆)

Melting Point: Mp 140°

pKa Value: pK_{a1} 4.28; pK_{a2} 5.34 (25°)

Other Data: Above Mp → anhydride

Aldrich: 19126-4

>>Derivative: Mono-Me ester, ((±)-)

CAS Registry Number: 132015-40-8

Molecular Formula: C₁₂H₁₄O₄

Molecular Weight: 222.24

Accurate Mass: 222.08921

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

Physical Description: Solid

Melting Point: Mp 94-95°

>>Derivative: Di-Me ester

CAS Registry Number: 19006-47-4

Molecular Formula: C₁₃H₁₆O₄

Molecular Weight: 236.267

Accurate Mass: 236.10486

Percentage Composition: C 66.09%; H 6.83%; O 27.09%

Physical Description: Prisms or needles (MeOH)

Melting Point: Mp 86-87°

Rare Chemicals Library: S50934-5

>>Derivative: Dichloride

Molecular Formula: C₁₁H₁₀Cl₂O₂

Molecular Weight: 245.104

Accurate Mass: 244.005784

Percentage Composition: C 53.90%; H 4.11%; Cl 28.93%; O 13.06%

Melting Point: Mp 46°

Boiling Point: Bp₁₈ 178-180°

>>Derivative: Monoamide, ((±)-)

CAS Registry Number: 131906-09-7

Molecular Formula: C₁₁H₁₃NO₃

Molecular Weight: 207.229

Accurate Mass: 207.089544

Percentage Composition: C 63.76%; H 6.32%; N 6.76%; O 23.16%

Physical Description: Powder

Melting Point: Mp 163-164°

>>Derivative: Diamide

CAS Registry Number: 78533-83-2

Molecular Formula: C₁₁H₁₄N₂O₂

Molecular Weight: 206.244

Accurate Mass: 206.105528

Percentage Composition: C 64.06%; H 6.84%; N 13.58%; O 15.52%

Physical Description: Cryst. (PhNO₂)

Melting Point: Mp 183-185°

Rare Chemicals Library: S59531-4