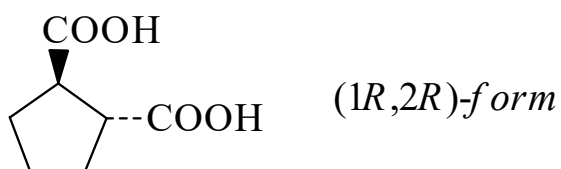




>>Entry Name: 1,2-Cyclopentanedicarboxylic acid, 9CI



CAS Registry Number: 50483-99-3

Related CAS Registry Numbers(s): 5763-49-5 30689-38-4 57287-23-7

Molecular Formula: C₇H₁₀O₄

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

>>Variant: (1*R*,2*R*)-form

Synonym(s): (–)-*trans*-form

CAS Registry Number: 17224-73-6

Molecular Formula: C₇H₁₀O₄

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 180-181°

Optical Rotation: [α]_D –85.9 (H₂O)

>>Derivative: Di-Et ester

Molecular Formula: C₁₁H₁₈O₄

Molecular Weight: 214.261

Accurate Mass: 214.12051

Percentage Composition: C 61.66%; H 8.47%; O 29.87%

Boiling Point: Bp₁₀₀ 170°

Optical Rotation: [α]_D –69.8 (Me₂CO)

>>Variant: (1*S*,2*S*)-form

Synonym(s): (+)-*trans*-form

CAS Registry Number: 21917-20-4

Molecular Formula: C₇H₁₀O₄

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 181°

Optical Rotation: [α]_D +87.6 (H₂O)

>>Derivative: Di-Et ester

Boiling Point: Bp₁₀₀ 170°

Optical Rotation: [α]_D +70.3 (Me₂CO)

>>Variant: (1*RS*,2*RS*)-form

Synonym(s): (±)-*trans*-form

CAS Registry Number: 1461-97-8

Molecular Formula: C₇H₁₀O₄

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Physical Description: Cryst.

Melting Point: Mp 162-163°

Solubility: Sol. hot H₂O

pKa Value: p*K*_{a1} 4.14; p*K*_{a2} 5.99 (20°)

Aldrich: 23756-6

Sigma: C9149