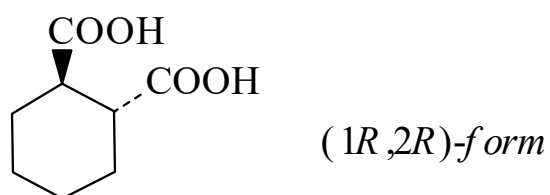




>>Entry Name: 1,2-Cyclohexanedicarboxylic acid, 9CI

Synonym(s): Hexahydrophthalic acid



CAS Registry Number: 1687-30-5

Related CAS Registry Numbers(s): 2305-32-0 2484-60-8 3205-35-4 31982-85-1 52782-07-7 71749-03-6 97233-90-4

Molecular Formula: C₈H₁₂O₄

Molecular Weight: 172.18

Accurate Mass: 172.07356

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

>>Derivative: Anhydride

Synonym(s): Hexahydro-1,3-isobenzofurandione, 9CI. Hexahydrophthalic anhydride

CAS Registry Number: 85-42-7

Molecular Formula: C₈H₁₀O₃

Molecular Weight: 154.165

Accurate Mass: 154.062995

Percentage Composition: C 62.33%; H 6.54%; O 31.13%

Use/Importance: Curing agent for epoxy resins. Intermed. for alkyd resins

Other Data: Unspecified mixt. of isomers

Aldrich: 12346-3

Rare Chemicals Library: S41930-3

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

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

CAS Registry Number: 46022-05-3

Molecular Formula: C₈H₁₂O₄

Molecular Weight: 172.18

Accurate Mass: 172.07356

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

Physical Description: Cryst. powder (H₂O)

Melting Point: Mp 179-183°

Optical Rotation: [α]_D -18.5

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

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

CAS Registry Number: 21963-41-7

Molecular Formula: C₈H₁₂O₄

Molecular Weight: 172.18

Accurate Mass: 172.07356

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

Use/Importance: Optically active polyamides with dicarboxylic acids are used for chromatog. optical resoln. of enantiomers

Physical Description: Cryst. powder (H₂O)

Melting Point: Mp 179-183°

Optical Rotation: [α]_D +18.2

Solubility: More sol. than the (±)-form

>>Derivative: Mono-Me ester

Molecular Formula: C₉H₁₄O₄

Molecular Weight: 186.207

Accurate Mass: 186.08921

Percentage Composition: C 58.05%; H 7.58%; O 34.37%

Melting Point: Mp 39°

Optical Rotation: [α]_D +26.5