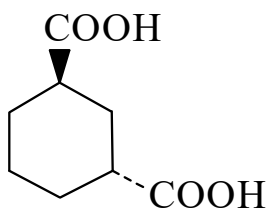




>>Entry Name: 1,3-Cyclohexanedicarboxylic acid, 9CI

Synonym(s): Hexahydroisophthalic acid



(1*R* ,3*R*)-*f*orm

CAS Registry Number: 3971-31-1

Related CAS Registry Numbers(s): 2888-58-6 7027-27-2 55467-96-4 62638-06-6

Molecular Formula: C₈H₁₂O₄

Molecular Weight: 172.18

Accurate Mass: 172.07356

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

Aldrich: 37543-8

>>Variant: (1*R*,3*R*)-form

Synonym(s): (–)-*trans*-form

Molecular Formula: C₈H₁₂O₄

Molecular Weight: 172.18

Accurate Mass: 172.07356

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

Melting Point: Mp 134°

Optical Rotation: [α]_D²² –23.1

>>Variant: (1*S*,3*S*)-form

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

Molecular Formula: C₈H₁₂O₄

Molecular Weight: 172.18

Accurate Mass: 172.07356

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

Melting Point: Mp 134°

Optical Rotation: [α]_D²² +23.46

>>Variant: (1*RS*,3*RS*)-form

Synonym(s): (±)-*trans*-form

CAS Registry Number: 2305-30-8

Molecular Formula: C₈H₁₂O₄

Molecular Weight: 172.18

Accurate Mass: 172.07356

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

Physical Description: Needles (H₂O)

Melting Point: Mp 150.5-150.7° (147-150°)

Solubility: Sol. hot H₂O

pKa Value: p*K*_a 4.86 (25°)

Other Data: Heat with AcCl → anhydride of *cis*-form

>>Derivative: Di-Me ester

CAS Registry Number: 10021-92-8

Molecular Formula: C₁₀H₁₆O₄

Molecular Weight: 200.234

Accurate Mass: 200.10486

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Boiling Point: Bp₂₀ 139°