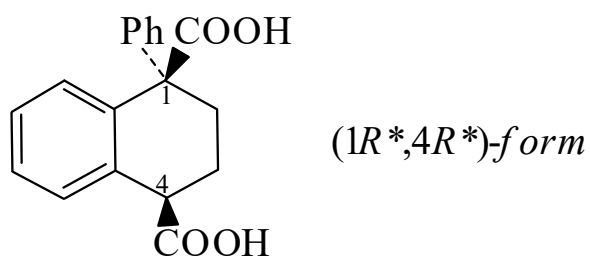




>>Entry Name: 1,2,3,4-Tetrahydro-1-phenyl-1,4-naphthalenedicarboxylic acid, 9CI

Synonym(s): Isatropic acid



Molecular Formula: C₁₈H₁₆O₄

Molecular Weight: 296.322

Accurate Mass: 296.10486

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

>>Variant: (1*R**,4*R**)-form

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

Molecular Formula: C₁₈H₁₆O₄

Molecular Weight: 296.322

Accurate Mass: 296.10486

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Melting Point: Mp 196.5-197.5°

Optical Rotation: [α]_D +8.95 (EtOH)

>>Variant: (1*S**,4*S**)-form

Synonym(s): (–)-*cis*-form

Molecular Formula: C₁₈H₁₆O₄

Molecular Weight: 296.322

Accurate Mass: 296.10486

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Melting Point: Mp 196.5-197°

Optical Rotation: [α]_D –8.8 (EtOH)

>>Variant: (1*R**S*,4*R**S*)-form

Synonym(s): (±)-*cis*-form. β-Isatropic acid

CAS Registry Number: 596-56-5

Molecular Formula: C₁₈H₁₆O₄

Molecular Weight: 296.322

Accurate Mass: 296.10486

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Physical Description: Plates (H₂O)

Melting Point: Mp 208.5-209°

pKa Value: p*K*_a 3.07

Other Data: Heat to 220-5° → α isomer

>>Derivative: Mono-Et ester

Molecular Formula: C₂₀H₂₀O₄

Molecular Weight: 324.376

Accurate Mass: 324.13616

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Melting Point: Mp 116°

>>Variant: (1*R**,4*S**)-form

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

Molecular Formula: C₁₈H₁₆O₄

Molecular Weight: 296.322

Accurate Mass: 296.10486

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Melting Point: Mp 239 dec.°

Optical Rotation: [α]_D²⁰ +9.44 (EtOH)

pKa Value: p*K*_a 3.92