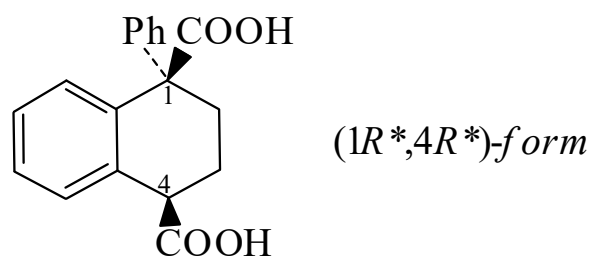




>>Entry Name: 1,2,3,4-Tetrahydro-1-phenyl-1,4-naphthalenedicarboxylic acid, 9CI

Synonym(s): Isatropic acid



**Molecular Formula:** C<sub>18</sub>H<sub>16</sub>O<sub>4</sub>

**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:** C<sub>18</sub>H<sub>16</sub>O<sub>4</sub>

**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]<sub>D</sub> +8.95 (EtOH)

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

Synonym(s): (–)-*cis*-form

**Molecular Formula:** C<sub>18</sub>H<sub>16</sub>O<sub>4</sub>

**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]<sub>D</sub> –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:** C<sub>18</sub>H<sub>16</sub>O<sub>4</sub>

**Molecular Weight:** 296.322

**Accurate Mass:** 296.10486

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

**Physical Description:** Plates (H<sub>2</sub>O)

**Melting Point:** Mp 208.5-209°

**pKa Value:** p*K*<sub>a</sub> 3.07

**Other Data:** Heat to 220-5° → α isomer

>>Derivative: Mono-Et ester

**Molecular Formula:** C<sub>20</sub>H<sub>20</sub>O<sub>4</sub>

**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:** C<sub>18</sub>H<sub>16</sub>O<sub>4</sub>

**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]<sub>D</sub><sup>20</sup> +9.44 (EtOH)

**pKa Value:** p*K*<sub>a</sub> 3.92