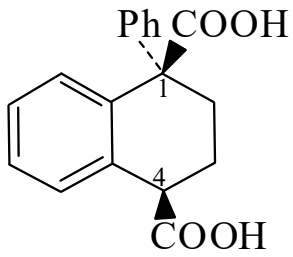
>>**Entry Name: 1,2,3,4-Tetrahydro-1-phenyl-1,4-naphthalenedicarboxylic acid,** 9CI
Synonym(s): Isatropic acid



(1*R**,4*R**)-*form*

Molecular Formula: $C_{18}H_{16}O_4$
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: $C_{18}H_{16}O_4$
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: $[\alpha]_D$ +8.95 (EtOH)

>>**Variant:** (1*S**,4*S**)-form
Synonym(s): (–)-*cis*-form

Molecular Formula: $C_{18}H_{16}O_4$
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: $[\alpha]_D$ –8.8 (EtOH)

>>**Variant:** (1*RS*,4*RS*)-form
Synonym(s): (±)-*cis*-form. β-Isatropic acid

CAS Registry Number: 596-56-5
Molecular Formula: $C_{18}H_{16}O_4$
Molecular Weight: 296.322
Accurate Mass: 296.10486
Percentage Composition: C 72.96%; H 5.44%; O 21.60%
Physical Description: Plates (H_2O)
Melting Point: Mp 208.5-209°
pKa Value: pK_a 3.07
Other Data: Heat to 220-5° → α isomer

>>**Derivative:** Mono-Et ester

Molecular Formula: $C_{20}H_{20}O_4$
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: $C_{18}H_{16}O_4$
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: $[\alpha]_D^{20}$+9.44 (EtOH)
pKa Value: pK_a 3.92