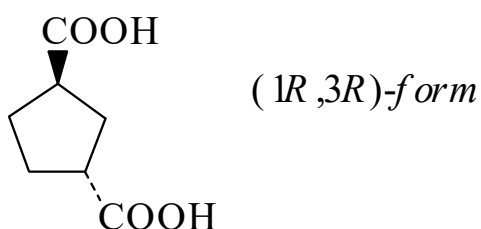




>>Entry Name: 1,3-Cyclopentanedicarboxylic acid, 9CI

Synonym(s): Norcamphoric acid



CAS Registry Number: 4056-78-4

Molecular Formula: $C_7H_{10}O_4$

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Hazard & Toxicity: Eye and skin irritant. LD₅₀ (rat, orl) 3250 mg/kg

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

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

CAS Registry Number: 36010-90-9

Molecular Formula: $C_7H_{10}O_4$

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Melting Point: Mp 93°

Optical Rotation: $[\alpha]_D -5.29$ (H₂O)

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

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

CAS Registry Number: 36010-89-6

Molecular Formula: $C_7H_{10}O_4$

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Melting Point: Mp 93.5°

Optical Rotation: $[\alpha]_D +5.86$ (H₂O)

>>Derivative: Mono-Et ester

Molecular Formula: $C_9H_{14}O_4$

Molecular Weight: 186.207

Accurate Mass: 186.08921

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

Boiling Point: Bp₂₀ 145°

Optical Rotation: $[\alpha]_D +5.01$

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

Synonym(s): (±)-trans-form

CAS Registry Number: 826-02-8

Molecular Formula: $C_7H_{10}O_4$

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Physical Description: Prisms (CCl₄)

Melting Point: Mp 88°

pKa Value: pK_a 4.3