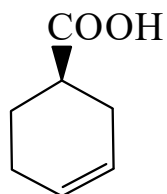




>>Entry Name: 3-Cyclohexene-1-carboxylic acid, 9CI

Synonym(s): Δ^3 -Tetrahydrobenzoic acid



(*R*)-form

CAS Registry Number: 4771-80-6

Molecular Formula: C₇H₁₀O₂

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Rare Chemicals Library: S43692-5

>>Variant: (*R*)-form

CAS Registry Number: 5709-98-8

Molecular Formula: C₇H₁₀O₂

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Physical Description: Oil

Boiling Point: Bp_{0.01} 63.5-66°

Optical Rotation: [α]_D +94.5 (c, 7 in EtOH)

>>Variant: ($\pm$)-form

Molecular Formula: C₇H₁₀O₂

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Melting Point: Mp 17°

Boiling Point: Bp₇₄₅ 237°. Bp₂₀ 132.5-133°

Hazard & Toxicity: Severe eye and skin irritant

>>Derivative: Me ester

CAS Registry Number: 6493-77-2

Molecular Formula: C₈H₁₂O₂

Molecular Weight: 140.182

Accurate Mass: 140.08373

Percentage Composition: C 68.55%; H 8.63%; O 22.83%

Boiling Point: Bp₂₀ 80°

Other: PB M15055

>>Derivative: Et ester

CAS Registry Number: 15111-56-5

Molecular Formula: C₉H₁₄O₂

Molecular Weight: 154.208

Accurate Mass: 154.09938

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Boiling Point: Bp 194-195°

>>Derivative: Nitrile

Synonym(s): 4-Cyanocyclohexene

CAS Registry Number: 100-45-8

Molecular Formula: C₇H₉N

Molecular Weight: 107.155

Accurate Mass: 107.073499

Percentage Composition: C 78.46%; H 8.47%; N 13.07%

Boiling Point: Bp 192-196°. Bp₂₅ 89-91°

Density: d₄²⁰ 0.96