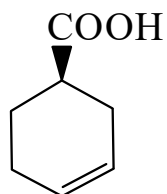




>>Entry Name: 3-Cyclohexene-1-carboxylic acid, 9CI

Synonym(s): Δ^3 -Tetrahydrobenzoic acid



(R)-form

CAS Registry Number: 4771-80-6

Molecular Formula: $C_7H_{10}O_2$

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: $C_7H_{10}O_2$

Molecular Weight: 126.155

Accurate Mass: 126.06808

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

Physical Description: Oil

Boiling Point: $B_{p0.01}$ 63.5-66°

Optical Rotation: $[\alpha]_D$ +94.5 (c, 7 in EtOH)

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

Molecular Formula: $C_7H_{10}O_2$

Molecular Weight: 126.155

Accurate Mass: 126.06808

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

Melting Point: M_p 17°

Boiling Point: B_{p745} 237°. B_{p20} 132.5-133°

Hazard & Toxicity: Severe eye and skin irritant

>>Derivative: Me ester

CAS Registry Number: 6493-77-2

Molecular Formula: $C_8H_{12}O_2$

Molecular Weight: 140.182

Accurate Mass: 140.08373

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

Boiling Point: B_{p20} 80°

Other: PB M15055

>>Derivative: Et ester

CAS Registry Number: 15111-56-5

Molecular Formula: $C_9H_{14}O_2$

Molecular Weight: 154.208

Accurate Mass: 154.09938

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

Boiling Point: B_p 194-195°

>>Derivative: Nitrile

Synonym(s): 4-Cyanocyclohexene

CAS Registry Number: 100-45-8

Molecular Formula: C_7H_9N

Molecular Weight: 107.155

Accurate Mass: 107.073499

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

Boiling Point: B_p 192-196°. B_{p25} 89-91°

Density: d_4^{20} 0.96