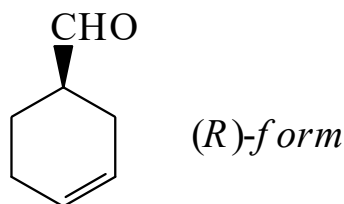




>>Entry Name: 3-Cyclohexene-1-carboxaldehyde, 9CI

Synonym(s): 1,2,3,6-Tetrahydrobenzaldehyde. Δ^3 -Tetrahydrobenzaldehyde. 4-Formylcyclohexene



Molecular Formula: $C_7H_{10}O$

Molecular Weight: 110.155

Accurate Mass: 110.073165

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

>>Variant: (R)-form

CAS Registry Number: 60631-76-7

Molecular Formula: $C_7H_{10}O$

Molecular Weight: 110.155

Accurate Mass: 110.073165

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Optical Rotation: $[\alpha]_D^{+95}$ (c, 3 in $CHCl_3$)

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

CAS Registry Number: 100-50-5

Molecular Formula: $C_7H_{10}O$

Molecular Weight: 110.155

Accurate Mass: 110.073165

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Physical Description: Oil

Melting Point: Mp -96.1°

Boiling Point: Bp 163.5 - 164.5° . Bp₁₃ 51 - 52°

Other Data: Polymerises very readily

Hazard & Toxicity: Flammable, fl. p. 57° (oc). Eye, skin and mucous membrane irritant. LD₅₀ (rat, orl) 2460 mg/kg

Aldrich: T1220-3

Fluka: 87320

>>Derivative: Oxime

CAS Registry Number: 4736-13-4

Molecular Formula: $C_7H_{11}NO$

Molecular Weight: 125.17

Accurate Mass: 125.084064

Percentage Composition: C 67.17%; H 8.86%; N 11.19%; O 12.78%

Physical Description: 2 forms, oil and cryst.

Melting Point: Mp 75 - 76° (cryst.)

Boiling Point: Bp₂₅ 128 - 129° (oil)

>>Derivative: Semicarbazone

Physical Description: Cryst. (C_6H_6 /petrol or MeOH aq.)

Melting Point: Mp 153.5 - 154.5°

>>Derivative: Phenylhydrazone

Boiling Point: Bp₂₂ 207 - 208°

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