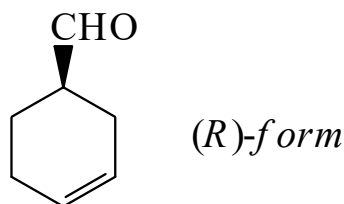




>>Entry Name: 3-Cyclohexene-1-carboxaldehyde, 9CI

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



Molecular Formula: C₇H₁₀O

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: C₇H₁₀O

Molecular Weight: 110.155

Accurate Mass: 110.073165

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

Optical Rotation: [α]_D +95 (c, 3 in CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 100-50-5

Molecular Formula: C₇H₁₀O

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: C₇H₁₁NO

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. (C₆H₆/petrol or MeOH aq.)

Melting Point: Mp 153.5-154.5°

>>Derivative: Phenylhydrazone

Boiling Point: Bp₂₂ 207-208°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 745B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 476D, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 567D, (ir)

Sobecki, W., *Ber.*, 1910, **43**, 1040, (synth)

Diels, O. *et al.*, *Annalen*, 1928, **460**, 121, (synth)

Org. Synth., 1971, **51**, 11, (synth)

Ceder, O. *et al.*, *Synth. Commun.*, 1976, **6**, 381, (synth)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, FNK025