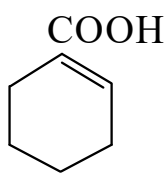




>>Entry Name: 1-Cyclohexene-1-carboxylic acid, 9CI

Synonym(s):  $\Delta^1$ -Tetrahydrobenzoic acid



CAS Registry Number: 636-82-8

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: Plates

Melting Point: Mp 38°

Boiling Point: Bp<sub>683</sub> 238-240°. Bp<sub>3</sub> 107°

Aldrich: 32836-7

>>Derivative: Me ester

CAS Registry Number: 18448-47-0

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%

Use/Importance: Synthetic reagent

Boiling Point: Bp 193.5-194.5°

Aldrich: 23218-1

Fluka: 29253

Sigma: C2547

>>Derivative: Chloride

CAS Registry Number: 36278-22-5

Molecular Formula:  $C_7H_9ClO$

Molecular Weight: 144.6

Accurate Mass: 144.034192

Percentage Composition: C 58.14%; H 6.27%; Cl 24.52%; O 11.06%

Boiling Point: Bp<sub>11</sub> 86°

>>Derivative: Amide

CAS Registry Number: 22546-81-2

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: Prisms (EtOH aq.), needles (EtOAc/hexane)

Melting Point: Mp 130-132° (127-128°)

>>Derivative: Nitrile

CAS Registry Number: 1855-63-6

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: Bp<sub>12</sub> 81°

Fluka: 29252

Rare Chemicals Library: S13409-0

References: