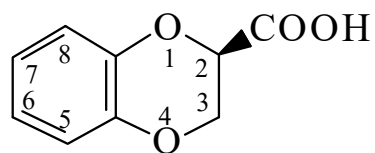




>>Entry Name: 1,4-Benzodioxan-2-carboxylic acid, 8Cl

Synonym(s): 2,3-Dihydro-1,4-benzodioxin-2-carboxylic acid, 9Cl



(R)-form

CAS Registry Number: 3663-80-7

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

>>Variant: (R)-form

CAS Registry Number: 70918-53-5

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Physical Description: Cryst. (toluene)

Melting Point: Mp 98-99°

Optical Rotation: $[\alpha]_D^{20} +62.1$ (c, 1 in CHCl₃)

Fluka: 12348

>>Variant: (±)-form

CAS Registry Number: 34385-93-8

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 125-126°

>>Derivative: K salt

Physical Description: Cryst. (EtOH)

Melting Point: Mp 198-202 dec.°

>>Derivative: Me ester

CAS Registry Number: 3663-79-4

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Melting Point: Mp 51-53°

Boiling Point: Bp₃ 136-137°

>>Derivative: Chloride

CAS Registry Number: 3663-81-8

Molecular Formula: C₉H₇ClO₃

Molecular Weight: 198.605

Accurate Mass: 198.008372

Percentage Composition: C 54.43%; H 3.55%; Cl 17.85%; O 24.17%

Physical Description: Needles

Melting Point: Mp 56-57°

Boiling Point: Bp₂ 122-123°