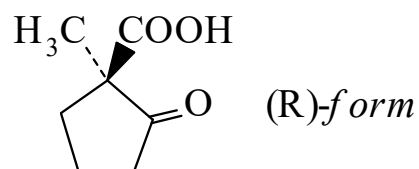




>>Entry Name: 1-Methyl-2-oxocyclopentanecarboxylic acid, 9CI

Synonym(s): 2-Methylcyclopentanone-2-carboxylic acid



CAS Registry Number: 50882-18-3

Related CAS Registry Numbers(s): 5453-88-3 64701-58-2

Molecular Formula: C₇H₁₀O₃

Molecular Weight: 142.154

Accurate Mass: 142.062995

Percentage Composition: C 59.14%; H 7.09%; O 33.76%

>>Variant: (R)-form

Molecular Formula: C₇H₁₀O₃

Molecular Weight: 142.154

Accurate Mass: 142.062995

Percentage Composition: C 59.14%; H 7.09%; O 33.76%

>>Derivative: Me ester

Molecular Formula: C₈H₁₂O₃

Molecular Weight: 156.181

Accurate Mass: 156.078645

Percentage Composition: C 61.52%; H 7.74%; O 30.73%

Optical Rotation: $[\alpha]_{\text{D}}^{23} -10.6$ (c, 1.15 in CHCl₃)

>>Derivative: Et ester

Molecular Formula: C₉H₁₄O₃

Molecular Weight: 170.208

Accurate Mass: 170.094295

Percentage Composition: C 63.51%; H 8.29%; O 28.20%

Physical Description: Oil

Boiling Point: Bp_{7.5} 96°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -13.3$ (c, 1.09 in CHCl₃)

>>Variant: (S)-form

Molecular Formula: C₇H₁₀O₃

Molecular Weight: 142.154

Accurate Mass: 142.062995

Percentage Composition: C 59.14%; H 7.09%; O 33.76%

>>Derivative: Et ester

CAS Registry Number: 72763-85-0

Melting Point: Mp 181°

Boiling Point: Bp₁₄ 101-102°

Optical Rotation: $[\alpha]_{\text{D}}^{22} +1.7$ (c, 10.33 in CHCl₃)

>>Variant: (±)-form

Molecular Formula: C₇H₁₀O₃

Molecular Weight: 142.154

Accurate Mass: 142.062995

Percentage Composition: C 59.14%; H 7.09%; O 33.76%

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Orange prisms (MeOH)

Melting Point: Mp 97-98°

Other Data: Sinters at 90°