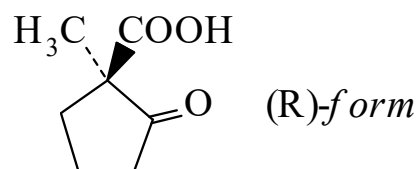




>>Entry Name: 1-Methyl-2-oxocyclopentanecarboxylic acid, 9CI

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:  $C_7H_{10}O_3$

Molecular Weight: 142.154

Accurate Mass: 142.062995

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

>>Variant: (R)-form

Molecular Formula:  $C_7H_{10}O_3$

Molecular Weight: 142.154

Accurate Mass: 142.062995

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

>>Derivative: Me ester

Molecular Formula:  $C_8H_{12}O_3$

Molecular Weight: 156.181

Accurate Mass: 156.078645

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

Optical Rotation:  $[\alpha]_D^{23} -10.6$  (c, 1.15 in  $CHCl_3$ )

>>Derivative: Et ester

Molecular Formula:  $C_9H_{14}O_3$

Molecular Weight: 170.208

Accurate Mass: 170.094295

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

Physical Description: Oil

Boiling Point:  $Bp_{7.5} 96^\circ$

Optical Rotation:  $[\alpha]_D^{20} -13.3$  (c, 1.09 in  $CHCl_3$ )

>>Variant: (S)-form

Molecular Formula:  $C_7H_{10}O_3$

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:  $Mp 181^\circ$

Boiling Point:  $Bp_{14} 101-102^\circ$

Optical Rotation:  $[\alpha]_D^{22} +1.7$  (c, 10.33 in  $CHCl_3$ )

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

Molecular Formula:  $C_7H_{10}O_3$

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:  $Mp 97-98^\circ$

Other Data: Sinters at  $90^\circ$