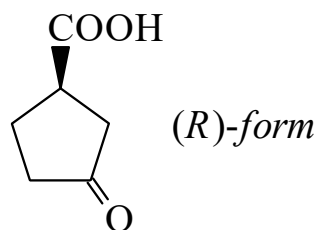




>>Entry Name: 3-Oxocyclopentanecarboxylic acid, 9CI



CAS Registry Number: 98-78-2

Related CAS Registry Numbers(s): 62646-11-1

Molecular Formula: C₆H₈O₃

Molecular Weight: 128.127

Accurate Mass: 128.047345

Percentage Composition: C 56.25%; H 6.29%; O 37.46%

Use/Importance: Intermed. for agrochemicals

>>Variant: (R)-form

CAS Registry Number: 13012-38-9

Molecular Formula: C₆H₈O₃

Molecular Weight: 128.127

Accurate Mass: 128.047345

Percentage Composition: C 56.25%; H 6.29%; O 37.46%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 65-67°

Boiling Point: Bp₄ 138-141°

Optical Rotation: [α]_D²³+22 (c, 1.5 in MeOH)

>>Derivative: Et ester

Molecular Formula: C₈H₁₂O₃

Molecular Weight: 156.181

Accurate Mass: 156.078645

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

Boiling Point: Bp₁₀ 90-91°

Optical Rotation: [α]_D²¹+20.8 (c, 2.5 in MeOH)

>>Variant: (±)-form

Molecular Formula: C₆H₈O₃

Molecular Weight: 128.127

Accurate Mass: 128.047345

Percentage Composition: C 56.25%; H 6.29%; O 37.46%

Melting Point: Mp 65-66°

Boiling Point: Bp₃₀ 197°

pKa Value: pK_{a1} 4.25 (20°)

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 149-150°

>>Derivative: Semicarbazone

Physical Description: Cryst. (H₂O)

Melting Point: Mp 197-198 dec.°

References:

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Sato, Y. *et al.*, *Chem. Pharm. Bull.*, 1963, **11**, 829, (*synth*)

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