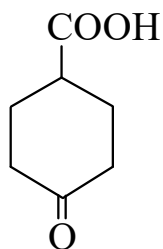




>>Entry Name: 4-Oxocyclohexanecarboxylic acid, 9CI

Synonym(s): Cyclohexanone-4-carboxylic acid



CAS Registry Number: 874-61-3

Molecular Formula: C₇H₁₀O₃

Molecular Weight: 142.154

Accurate Mass: 142.062995

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

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 68°

Boiling Point: Bp₃₀ 210°

pKa Value: pK_a 4.38

>>Derivative: Me ester

CAS Registry Number: 6297-22-9

Molecular Formula: C₈H₁₂O₃

Molecular Weight: 156.181

Accurate Mass: 156.078645

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

Boiling Point: Bp₂₀ 140°

>>Derivative: Et ester

CAS Registry Number: 17159-79-4

Molecular Formula: C₉H₁₄O₃

Molecular Weight: 170.208

Accurate Mass: 170.094295

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

Physical Description: Cryst.

Melting Point: Mp 67-68°

Boiling Point: Bp₄₀ 150-152°. Bp_{0.5} 70°

Aldrich: 32062-5

Fluka: 29160

>>Derivative: Oxime

Molecular Formula: C₇H₁₁NO₃

Molecular Weight: 157.169

Accurate Mass: 157.073894

Percentage Composition: C 53.49%; H 7.05%; N 8.91%; O 30.54%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 146-147°

References:

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