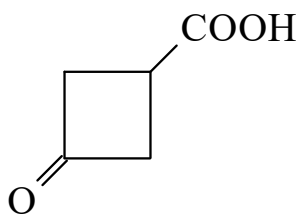




>>Entry Name: 3-Oxocyclobutanecarboxylic acid



CAS Registry Number: 23761-23-1

Molecular Formula: $C_5H_6O_3$

Molecular Weight: 114.101

Accurate Mass: 114.031695

Percentage Composition: C 52.63%; H 5.30%; O 42.07%

Physical Description: Needles (C_6H_6 /hexane)

Melting Point: Mp 69-70°

>>Derivative: *N,N*-Dimethylamide

Molecular Formula: $C_7H_{11}NO_2$

Molecular Weight: 141.169

Accurate Mass: 141.078979

Percentage Composition: C 59.56%; H 7.85%; N 9.92%; O 22.67%

Boiling Point: Bp₁ 108-111°

>>Derivative: Di-Me ketal, Me ester

Synonym(s): Methyl 3,3-dimethoxy-1-cyclobutanecarboxylate

Molecular Formula: $C_8H_{14}O_4$

Molecular Weight: 174.196

Accurate Mass: 174.08921

Percentage Composition: C 55.16%; H 8.10%; O 36.74%

Physical Description: Liq.

Boiling Point: Bp₈ 80-83°

>>Derivative: Di-Et ketal, *N,N*-dimethylamide

Molecular Formula: $C_{11}H_{21}NO_3$

Molecular Weight: 215.292

Accurate Mass: 215.152144

Percentage Composition: C 61.37%; H 9.83%; N 6.51%; O 22.29%

Boiling Point: Bp₁ 110°

>>Derivative: Ethylene ketal, *N,N*-dimethylamide

Molecular Formula: $C_9H_{15}NO_3$

Molecular Weight: 185.222

Accurate Mass: 185.105194

Percentage Composition: C 58.36%; H 8.16%; N 7.56%; O 25.91%

Boiling Point: Bp₁ 114°

References:

- Avram, M. *et al.*, *Chem. Ber.*, 1957, **90**, 1424, (*deriv, synth*)
Caserio, F.F. *et al.*, *J.A.C.S.*, 1958, **80**, 5837, (*synth, deriv*)
Pigou, P.E. *et al.*, *J.O.C.*, 1988, **53**, 3841, (*synth, pmr, cmr*)
Bashir-Hashemi, A. *et al.*, *J.O.C.*, 1994, **59**, 2132, (*synth, Me ester*)
Stevens, C. *et al.*, *J.O.C.*, 1996, **61**, 2174, (*deriv, synth, pmr, cmr, ms*)