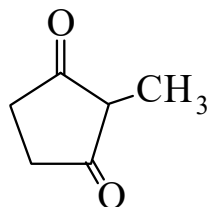




>>Entry Name: 2-Methyl-1,3-cyclopentanedione, 9CI
Synonym(s): 3-Hydroxy-2-methyl-2-cyclopenten-1-one



CAS Registry Number: 765-69-5

Molecular Formula: C₆H₈O₂
Molecular Weight: 112.128
Accurate Mass: 112.05243
Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Use/Importance: Intermed. in total synth. of steroids
Physical Description: Cryst. (EtOH aq.)
Melting Point: Mp 212-214°

Aldrich: 11702-1
Fluka: 66515
Sigma: M0394

>>Derivative: Dioxime

Molecular Formula: C₆H₁₀N₂O₂
Molecular Weight: 142.157
Accurate Mass: 142.074228
Percentage Composition: C 50.69%; H 7.09%; N 19.71%; O 22.51%
Melting Point: Mp 198 dec.°

>>Derivative: Monoethylene ketal

Synonym(s): 6-Methyl-1,4-dioxaspiro[4.4]nonan-7-one, 9CI

CAS Registry Number: 54972-03-1
Molecular Formula: C₈H₁₂O₃
Molecular Weight: 156.181
Accurate Mass: 156.078645
Percentage Composition: C 61.52%; H 7.74%; O 30.73%
Physical Description: Oil
Boiling Point: Bp_{0.01} 48°

>>Derivative: Bis(ethylene ketal)

Synonym(s): 6-Methyl-1,4,8,11-tetraoxadispiro[4.1.4.2]tridecane, 9CI

CAS Registry Number: 81770-72-1
Molecular Formula: C₁₀H₁₆O₄
Molecular Weight: 200.234
Accurate Mass: 200.10486
Percentage Composition: C 59.98%; H 8.05%; O 31.96%
Physical Description: Oil
Boiling Point: Bp_{0.01} 80°

References:

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 389D, (nmr)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 426D, (ir)
Schick, H. *et al.*, *Angew. Chem., Int. Ed.*, 1967, **6**, 80-81, (synth)
Miki, T. *et al.*, *Chem. Pharm. Bull.*, 1967, **15**, 670-673, (synth)
Grenda, V.J. *et al.*, *J.O.C.*, 1967, **32**, 1236-1237, (synth)
Org. Synth., Coll. Vol., 5, 1973, 747-751, (synth)
Volpe, T. *et al.*, *Tet. Lett.*, 1986, **27**, 2853-2854, (monoethylene ketal, synth, ir, pmr, cmr)
Katrusiak, A., *Acta Cryst. C*, 1989, **45**, 1897-1899, (cryst struct)
Martinez, R.A. *et al.*, *Synth. Commun.*, 1989, **19**, 373-377, (synth, pmr)
Org. Synth., Coll. Vol., 9, 1998, 570-572, (synth)