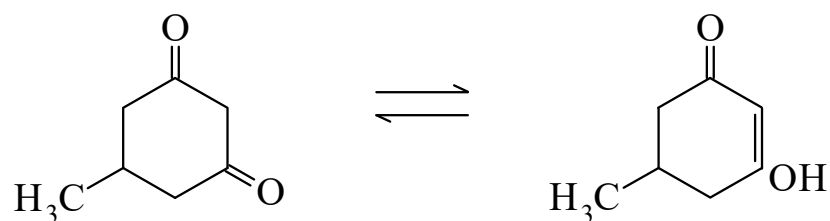




>>Entry Name: 5-Methyl-1,3-cyclohexanedione, 9CI

Synonym(s): 3-Hydroxy-5-methyl-2-cyclohexen-1-one



CAS Registry Number: 4341-24-6

Molecular Formula: $C_7H_{10}O_2$

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 126-127° (139-141°)

Boiling Point: Bp_{0.3} 60°

Solubility: Sol. hot H₂O

pKa Value: pK_a 5.24

Other Data: Mixt. of tautomers

Aldrich: 27995-1

Fluka: 66313

>>Derivative: Dioxime

CAS Registry Number: 41704-77-2

Molecular Formula: $C_7H_{12}N_2O_2$

Molecular Weight: 156.184

Accurate Mass: 156.089878

Percentage Composition: C 53.83%; H 7.74%; N 17.94%; O 20.49%

Physical Description: Prisms (H₂O), needles (EtOH)

Melting Point: Mp 155-157°

>>Derivative: Disemicarbazone

Physical Description: Amorph.

Other Data: Dec. at 225°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 703A, (nmr)

Kvita, V. *et al.*, *Coll. Czech. Chem. Comm.*, 1957, **22**, 1064, (synth)

Stork, G. *et al.*, *J.A.C.S.*, 1962, **84**, 310, (synth)

Szychowski, J. *et al.*, *Can. J. Chem.*, 1979, **57**, 1631, (synth)

Schinzer, D. *et al.*, *Annalen*, 1991, 139, (synth, pmr)

Edafiogho, I.O. *et al.*, *J. Med. Chem.*, 1992, **35**, 2798, (synth)