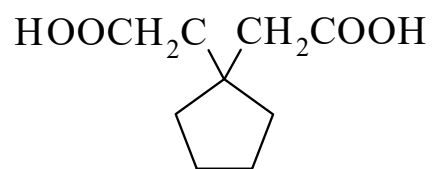




>>Entry Name: 1,1-Cyclopentanediacetic acid, 9CI

Synonym(s): 3,3-Tetramethyleneglutaric acid



CAS Registry Number: 16713-66-9

Molecular Formula: $\text{C}_9\text{H}_{14}\text{O}_4$

Molecular Weight: 186.207

Accurate Mass: 186.08921

Percentage Composition: C 58.05%; H 7.58%; O 34.37%

Melting Point: Mp 180-181°

pKa Value: $\text{p}K_{\text{a}1}$ 3.8; $\text{p}K_{\text{a}2}$ 6.77 (25°)

Aldrich: T2190-3

Sigma: T3385

>>Derivative: Di-Me ester

CAS Registry Number: 70197-60-3

Molecular Formula: $\text{C}_{11}\text{H}_{18}\text{O}_4$

Molecular Weight: 214.261

Accurate Mass: 214.12051

Percentage Composition: C 61.66%; H 8.47%; O 29.87%

Boiling Point: Bp_{17} 141°

>>Derivative: Anhydride

Synonym(s): 8-Oxaspiro[4.5]decane-7,9-dione, 9CI

CAS Registry Number: 5662-95-3

Molecular Formula: $\text{C}_9\text{H}_{12}\text{O}_3$

Molecular Weight: 168.192

Accurate Mass: 168.078645

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Melting Point: Mp 64-66°

Boiling Point: Bp_{15} 186°

Aldrich: T2195-4

Fluka: 87840

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 841C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 540C; 721C, (ir, anhydride)

Foos, J. *et al.*, *J.O.C.*, 1979, **44**, 2522, (synth)