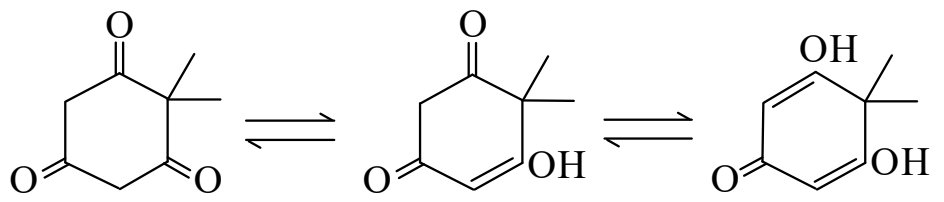
>>**Entry Name: 2,2-Dimethyl-1,3,5-cyclohexanetrione,** 9CI
Synonym(s): Filicinic acid



Trioxo-*form* Monoenol-*form* Dienediol-*form*

CAS Registry Number: 511-68-2
Type of Compound Code(s): VA2100 XA0900

Molecular Formula: $C_8H_{10}O_3$
Molecular Weight: 154.165
Accurate Mass: 154.062995
Percentage Composition: C 62.33%; H 6.54%; O 31.13%
Biological Source: Isol. from *Dryopteris* ferns
Use/Importance: Anthelmintic, bactericide
Physical Description: Prisms (H_2O or C_6H_6)
Melting Point: Mp 212-215°. Mp 215 dec., 220° dec.°
Solubility: Mod. sol. hot H_2O, hot EtOH, spar. sol. Et_2O, AcOH
pKa Value: pK_a 5.8 pK_{a1} 4.2; pK_{a2} 9.73 (25°)

>>**Variant:** Monoenol-form
Synonym(s): 5-Hydroxy-6,6-dimethyl-4-cyclohexene-1,3-dione, 9CI, 8CI

Molecular Formula: $C_8H_{10}O_3$
Molecular Weight: 154.165
Accurate Mass: 154.062995
Percentage Composition: C 62.33%; H 6.54%; O 31.13%

>>**Derivative:** Me ether
Synonym(s): 5-Methoxy-6,6-dimethoxy-4-cyclohexene-1,3-dione

Molecular Formula: $C_9H_{12}O_3$
Molecular Weight: 168.192
Accurate Mass: 168.078645
Percentage Composition: C 64.27%; H 7.19%; O 28.54%
Physical Description: Prisms (EtOAc)
Melting Point: Mp 205-207°
Boiling Point: Bp_{18} 194-196°

>>**Variant:** Dienediol-form
Synonym(s): 3,5-Dihydroxy-4,4-dimethyl-2,5-cyclohexadien-1-one

CAS Registry Number: 2065-00-1
Molecular Formula: $C_8H_{10}O_3$
Molecular Weight: 154.165
Accurate Mass: 154.062995
Percentage Composition: C 62.33%; H 6.54%; O 31.13%

>>**Derivative:** Di-Et ether
Synonym(s): 3,5-Diethoxy-4,4-dimethyl-2,5-cyclohexadien-1-one

Molecular Formula: $C_{12}H_{18}O_3$
Molecular Weight: 210.272
Accurate Mass: 210.125595
Percentage Composition: C 68.55%; H 8.63%; O 22.83%
Physical Description: Plates or prisms (petrol)
Melting Point: Mp 103-105°

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