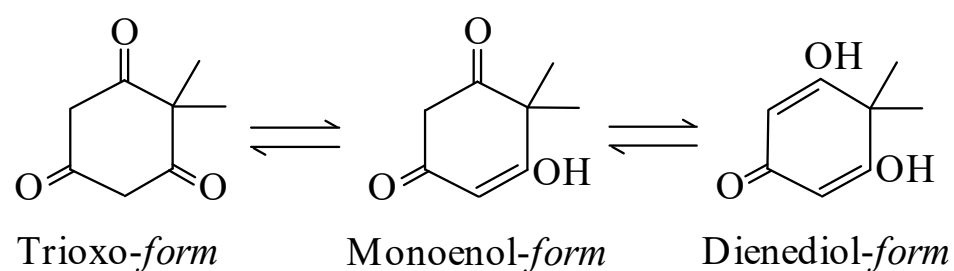




>>Entry Name: 2,2-Dimethyl-1,3,5-cyclohexanetrione, 9CI

Synonym(s): Filicinic acid



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°