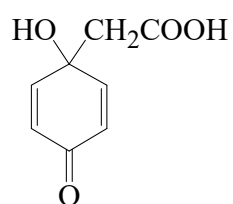




>>Entry Name: 1-Hydroxy-4-oxo-2,5-cyclohexadiene-1-acetic acid



CAS Registry Number: 55604-87-0

Molecular Formula: C₈H₈O₄

Molecular Weight: 168.149

Accurate Mass: 168.04226

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Biological Source: Constit. of *Pseudogynoxys cunninghamii*

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 103-104°

Solubility: BERDY SOL: Sol. Et₂O, MeOH; poorly sol. H₂O

Calculated Log P Data: Log P -0.69 (calc)

UV: [neutral] λ_{max} 226 (ε 14500) (EtOH) (Derep) [neutral] λ_{max} 220 (log ε 4.18) (EtOH) [neutral] λ_{max} 227 (ε 12500) (MeOH) (Berdy) [neutral] λ_{max} 225 (ε 15000) (EtOH) (Berdy)

>>Derivative: Me ester

Synonym(s): Jacaranone

CAS Registry Number: 60263-07-2

Molecular Formula: C₉H₁₀O₄

Molecular Weight: 182.176

Accurate Mass: 182.05791

Percentage Composition: C 59.34%; H 5.53%; O 35.13%

Biological Source: Constit. of *Ajuga parviflora*, *Cineraria* spp., *Jacaranda* spp., *Pseudogynoxys* spp. and *Senecio* spp.

Biological Use/Importance: Cytotoxic agent

Physical Description: Cryst. (CHCl₃/hexane)

Melting Point: Mp 80-81° (76-77°)

>>Derivative: Et ester

CAS Registry Number: 60263-06-1

Molecular Formula: C₁₀H₁₂O₄

Molecular Weight: 196.202

Accurate Mass: 196.07356

Percentage Composition: C 61.22%; H 6.16%; O 32.62%

Biological Source: Constit. of *Ajuga parviflora*, *Emilia* sp., *Jacaranda* and *Senecio* spp.

Biological Use/Importance: Cytotoxic agent

Physical Description: Cryst. (CHCl₃/hexane)

Melting Point: Mp 72-74°

>>Derivative: Di-Et acetal, amide

Synonym(s): 4,4-Diethoxy-1-hydroxy-2,5-cyclohexadiene-1-acetamide

CAS Registry Number: 253308-66-6

Molecular Formula: C₁₂H₁₉NO₄

Molecular Weight: 241.286

Accurate Mass: 241.131409

Percentage Composition: C 59.73%; H 7.94%; N 5.81%; O 26.52%

Biological Source: Isol. from the sponge *Verongia aerophoba*