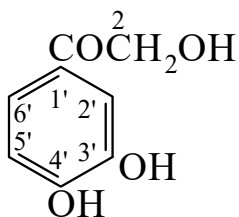




>>Entry Name: 2,3',4'-Trihydroxyacetophenone, 8Cl

Synonym(s): 1-(3,4-Dihydroxyphenyl)-2-hydroxyethanone, 9Cl. α ,3,4-Trihydroxyacetophenone. 3,4-Dihydroxyphenacyl alcohol



CAS Registry Number: 29477-54-1

Molecular Formula: $C_8H_8O_4$

Molecular Weight: 168.149

Accurate Mass: 168.04226

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

Biological Source: Found in insect cuticle

Use/Importance: Used as 1mM aq. soln. for photometric detn. of Ca ($\lambda_{\max}$ 540 nm, pH =11.5), Ba ($\lambda_{\max}$ 560 nm, pH 11.8-12.4)

Physical Description: Cryst. (H_2O)

Melting Point: Mp 195°

UV: [neutral] $\lambda_{\max}$ 220 (log ϵ 3.7); 231 (log ϵ 3.7); 290 (sh) (log ϵ 3.6); 325 (log ϵ 3.8) (MeOH)

>>Derivative: 3',4'-Di-Ac

Molecular Formula: $C_{12}H_{12}O_6$

Molecular Weight: 252.223

Accurate Mass: 252.06339

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

Physical Description: Plates (EtOH)

Melting Point: Mp 86-87°

>>Derivative: 2,3',4'-Tri-Ac

Molecular Formula: $C_{14}H_{14}O_7$

Molecular Weight: 294.26

Accurate Mass: 294.073955

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

Physical Description: Plates (MeOH)

Melting Point: Mp 95°

>>Derivative: 2-O-(3,4-Dihydroxy-*E*-cinnamoyl)

Synonym(s): Petasiphenone. 3,4-Dihydroxyphenacyl caffeate

CAS Registry Number: 162616-81-1

Molecular Formula: $C_{17}H_{14}O_7$

Molecular Weight: 330.293

Accurate Mass: 330.073955

Percentage Composition: C 61.82%; H 4.27%; O 33.91%

Biological Source: Constit. of the rhizomes of *Petasites japonicus*

Physical Description: Pale brown powder

Melting Point: Mp 236-238°

UV: [neutral] $\lambda_{\max}$ 220 (log ϵ 3.7); 231 (log ϵ 3.7); 290 (sh) (log ϵ 3.6); 325 (log ϵ 3.8) (MeOH)

>>Derivative: 3'-Me ether

Synonym(s): 2,4'-Dihydroxy-3'-methoxyacetophenone. α -Hydroxyacetovanillone

Molecular Formula: $C_9H_{10}O_4$

Molecular Weight: 182.176

Accurate Mass: 182.05791

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

Biological Source: Component of lignins of conifers and from *Lycopodium* spp.

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 109-110°