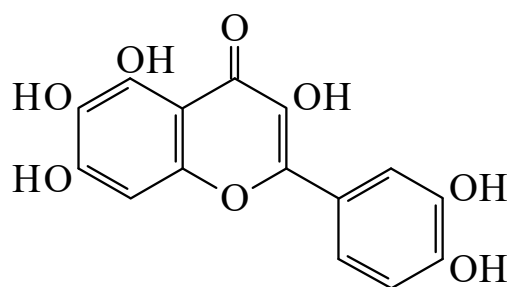




>>Entry Name: 3,3',4',5,6,7-Hexahydroxyflavone

Synonym(s): 2-(3,4-Dihydroxyphenyl)-3,5,6,7-tetrahydroxy-4*H*-1-benzopyran-4-one, 9Cl. 3',4',5,6,7-Pentahydroxyflavonol. **Quercetagetin**. 6-Hydroxyquercetin



CAS Registry Number: 90-18-6

Related CAS Registry Numbers(s): 100363-98-2

Molecular Formula: C₁₅H₁₀O₈

Molecular Weight: 318.239

Accurate Mass: 318.03757

Percentage Composition: C 56.61%; H 3.17%; O 40.22%

Biological Source: Isol. from *Tagetes*, *Artemisia*, *Achillea*, *Eupatorium* and other genera

Use/Importance: Used as 2mM soln. in EtOH for photometric detn. of Zr ($\lambda_{\max}$ 415 nm). Shows anti-HIV activity

Physical Description: Pale yellow cryst. + 2H₂O (EtOH aq.)

Melting Point: Mp 325° (318-320°)

Solubility: Sol. EtOH, alkalis; sl. sol. H₂O

Calculated Log P Data: Log P -0.88 (calc)

UV: [neutral] $\lambda_{\max}$ 259 (ϵ 16982); 361 (ϵ 21877) (MeOH) (Berdy)

>>Derivative: 3-*O*- α -L-Rhamnopyranoside

Synonym(s): Quercetagetin 3-rhamnoside

CAS Registry Number: 64543-29-9

Molecular Formula: C₂₁H₂₀O₁₂

Molecular Weight: 464.382

Accurate Mass: 464.09548

Percentage Composition: C 54.32%; H 4.34%; O 41.34%

Biological Source: Isol. from *Juniperus macropoda*

Melting Point: Mp 195°

>>Derivative: 3-*O*- β -D-Galactopyranoside

Synonym(s): Quercetagetin 3-galactoside

Molecular Formula: C₂₁H₂₀O₁₃

Molecular Weight: 480.381

Accurate Mass: 480.090395

Percentage Composition: C 52.51%; H 4.20%; O 43.30%

Biological Source: Isol. from *Rhododendron* sp. and *Lotus corniculatus*

Physical Description: Deep yellow prisms

Melting Point: Mp 200°

>>Derivative: 3-*O*- β -D-Glucopyranoside

Synonym(s): **Tagetiin**. Quercetagetin 3-glucoside

CAS Registry Number: 60671-81-0

Molecular Formula: C₂₁H₂₀O₁₃

Molecular Weight: 480.381

Accurate Mass: 480.090395

Percentage Composition: C 52.51%; H 4.20%; O 43.30%

Biological Source: Isol. from *Tagetes erecta*

Physical Description: Needles + 3H₂O

Melting Point: Mp 203 dec.° (195-198°)

Optical Rotation: $[\alpha]_D^{19}$ -109.6