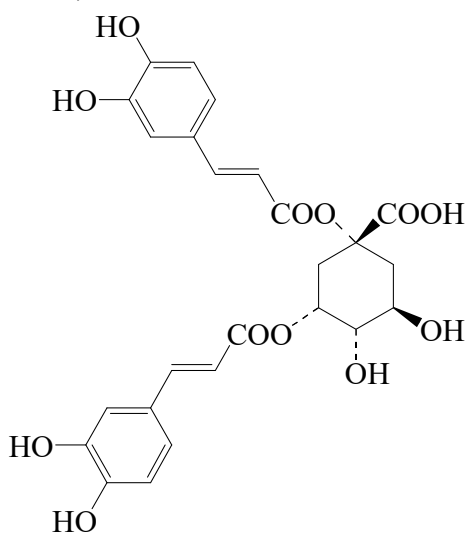




>>Entry Name: 1,5-Di-*O*-caffeoylquinic acid

Synonym(s): 1,5-Bis(3,4-dihydroxycinnamoyl)quinic acid. **Cynarine**, INN. Plemocil. Cinarcaf. Cinarina. CYN. Cynarex. Nivellipid. Listrocol



Related CAS Registry Numbers(s): 1884-24-8 19870-46-3

Molecular Formula: C₂₅H₂₄O₁₂

Molecular Weight: 516.457

Accurate Mass: 516.12678

Percentage Composition: C 58.14%; H 4.68%; O 37.17%

General Statement: Can also be numbered 1,3-dicaffeoyl. 1,5- is more usual. Has been confused in CAS with the 1,4-isomer

Rare Chemicals Library: S43025-0

>>Variant: (*E,E*)-form

Molecular Formula: C₂₅H₂₄O₁₂

Molecular Weight: 516.457

Accurate Mass: 516.12678

Percentage Composition: C 58.14%; H 4.68%; O 37.17%

Biological Source: Isol. from *Cyanara scolymus*, *Rhus typhina* flowers, *Senecio nemorensis* and *Cirsium arvense*

Biological Use/Importance: Choleric agent. Hepatoprotective activity *in vitro*

Physical Description: Cryst.

Melting Point: Mp 227-228°

Optical Rotation: $[\alpha]_D^{25} -59$ (c, 2 in MeOH)

UV: [neutral] $\lambda_{\max}$ 326 (E1%/1cm 616) (MeOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, ipr) 1900 mg/kg

>>Derivative: Hexa-Ac

CAS Registry Number: 30964-13-7

Molecular Formula: C₃₇H₃₆O₁₈

Molecular Weight: 768.681

Accurate Mass: 768.19017

Percentage Composition: C 57.81%; H 4.72%; O 37.47%

Physical Description: Cryst.

Melting Point: Mp 168-172°

>>Derivative: 3',3''-Di-Me ether

Synonym(s): 1,5-Di-*O*-feruloylquinic acid

Molecular Formula: C₂₇H₂₈O₁₂

Molecular Weight: 544.511

Accurate Mass: 544.15808

Percentage Composition: C 59.56%; H 5.18%; O 35.26%

Biological Source: Constit. of the roots of nutrient-deprived *Brachiaria decumbens* and *Brachiaria ruziziensis*

Physical Description: Pale yellow powder

UV: [neutral] $\lambda_{\max}$ 295 (sh) (); 330 (4.26); 388 (sh) () (H₂O)

References: