



>>Entry Name: 3,5-Di-*O*-caffeoylquinic acid

ENTRY UNDER REVIEW

Synonym(s): 3,5-Bis-(3,4-dihydroxycinnamoyl)quinic acid. Isochlorogenic acid a

CAS Registry Number: 2450-53-5

Molecular Formula: C₂₅H₂₄O₁₂

Molecular Weight: 516.457

Accurate Mass: 516.12678

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

General Statement: Care needed with numbering. Positions 3 and 5 frequently interchanged

Biological Source: Isol. from coffee and maté, globe artichoke (*Cyanara scolymus*) and caucasian whortleberry (*Vaccinium arctostaphylos*)

Physical Description: Cryst.

Melting Point: Mp 170-172 dec.°

Optical Rotation: [α]_D −198 (MeOH)

>>Derivative: Me ester

Synonym(s): Macroantoin G. Macranthoin G

CAS Registry Number: 159934-13-1

Molecular Formula: C₂₆H₂₆O₁₂

Molecular Weight: 530.484

Accurate Mass: 530.14243

Percentage Composition: C 58.87%; H 4.94%; O 36.19%

Biological Source: Constit. of *Lonicera macranthoides*

>>Derivative: 1-*O*-(2-Methylpropanoyl)

Synonym(s): 3,5-Dicaffeoyl-1-isobutyrylquinic acid

Molecular Formula: C₂₉H₃₀O₁₃

Molecular Weight: 586.548

Accurate Mass: 586.168645

Percentage Composition: C 59.38%; H 5.16%; O 35.46%

Biological Source: Constit. of the flowerheads of *Buphthalmum salicifolia*

Physical Description: Amorph. pale yellow powder

UV: [neutral] λ_{max} 242 (); 300 (sh) (); 328 () (MeOH)

>>Derivative: 4-*O*-(4-Carboxy-3-hydroxy-3-methylbutanoyl)

Synonym(s): 3,5-Dicaffeoyl-4-*O*-(3-hydroxy-3-methylglutaroyl)quinic acid

CAS Registry Number: 114637-82-0

Molecular Formula: C₃₁H₃₂O₁₆

Molecular Weight: 660.584

Accurate Mass: 660.16904

Percentage Composition: C 56.37%; H 4.88%; O 38.75%

Biological Source: Constit. of the fruit fly *Gardenia jasminoides*. Component of Zhi Zi

Physical Description: Amorph. powder +½H₂O

Optical Rotation: [α]_D²⁰ −170 (c, 0.95 in MeOH)

UV: [neutral] λ_{max} 216 (ε 26600); 242 (ε 17600); 304 (sh) (); 329 (ε 30800) (MeOH)

>>Derivative: 4-*O*-Succinoyl

Synonym(s): 3,5-Dicaffeoyl-4-succinoylquinic acid

CAS Registry Number: 179761-31-0

Molecular Formula: C₂₉H₂₈O₁₅

Molecular Weight: 616.531

Accurate Mass: 616.142825

Percentage Composition: C 56.50%; H 4.58%; O 38.93%

Biological Source: Constit. of *Chrysanthemum coronarium*

Use/Importance: Antioxidant