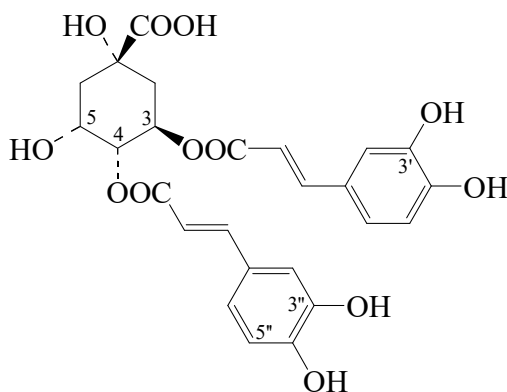




>>Entry Name: 3,4-Di-*O*-caffeoylquinic acid

ENTRY UNDER REVIEW

Synonym(s): Isochlorogenic acid b



CAS Registry Number: 14534-61-3

Related CAS Registry Numbers(s): 2271-12-7

Molecular Formula: C₂₅H₂₄O₁₂

Molecular Weight: 516.457

Accurate Mass: 516.12678

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

General Statement: Numbering systems vary

Biological Source: Isol. from coffee and maté

Physical Description: Powder

Melting Point: Mp 234-238 dec.°

Optical Rotation: $[\alpha]_D^{28} -225$ (MeOH)

>>Derivative: Me ester

Synonym(s): Macroantoin F, Macranthoin F

CAS Registry Number: 114637-83-1

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: 5-*O*-(3-Hydroxy-3-methylglutaroyl)

CAS Registry Number: 103744-76-9

Molecular Formula: C₃₁H₃₂O₁₆

Molecular Weight: 660.584

Accurate Mass: 660.16904

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

Biological Source: Isol. from fruit of *Gardenia jasminoides*

Biological Use/Importance: Lipxygenase inhibitor

Optical Rotation: $[\alpha]_D^{18} -169.8$ (c, 0.95 in MeOH)

>>Derivative: 3'-Me ether

Synonym(s): 4-*O*-Caffeoyl-3-*O*-feruloylquinic acid

CAS Registry Number: 96990-65-7

Extra CAS Registry Numbers(s): 102851-10-5

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 coffee beans