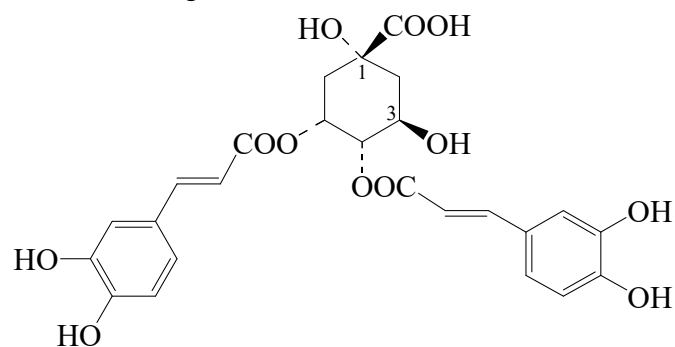




>>Entry Name: 4,5-Di-*O*-caffeoylquinic acid

ENTRY UNDER REVIEW

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



CAS Registry Number: 57378-72-0

Related CAS Registry Numbers(s): 32451-88-0

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, Brazilian propolis and maté

Physical Description: Cryst.

Melting Point: Mp 140 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{28} -170$ (MeOH)

References:

Scarpati, M.L. *et al.*, *Tet. Lett.*, 1964, 2851, (*isol*)

Timmermann, B.N. *et al.*, *J. Nat. Prod.*, 1983, **46**, 365-368, (*isol*, *pmr*, *cmr*)

Tatefuji, T. *et al.*, *Biol. Pharm. Bull.*, 1996, **19**, 966-970, (*isol*, *pmr*, *cmr*)

Miketova, P. *et al.*, *J. Mass Spectrom.*, 1999, **34**, 1240-1252, (*ms*)