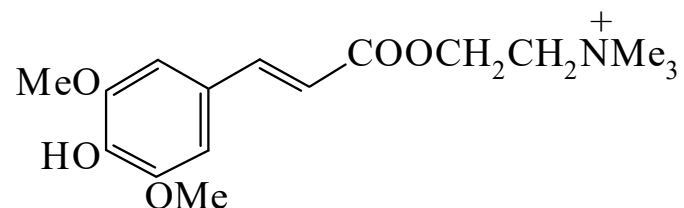




>>Entry Name: Sinapine

ENTRY UNDER REVIEW

Synonym(s): 2-[[3-(4-Hydroxy-3,5-dimethoxyphenyl)-1-oxo-2-propenyl]oxy]-*N,N,N*- trimethylethanaminium, 9Cl. Choline 4-hydroxy-3,5-dimethoxycinnamate, 8Cl



CAS Registry Number: 18696-26-9

Related CAS Registry Numbers(s): 84123-21-7 84123-22-8

Molecular Formula: C₁₆H₂₄NO₅⁽⁺⁾

Molecular Weight: 310.369

Accurate Mass: 310.165449

Percentage Composition: C 61.92%; H 7.79%; N 4.51%; O 25.77%

nemorosa) (Cruciferae)

Use/Importance: Astringent antinutrient of practical importance, esp. in cattle feed, e.g. rape meal. Reported to have radioprotective effects in some cruciferous plants and in *Drosophila*

>>Derivative: Iodide

CAS Registry Number: 5655-06-1

Molecular Formula: C₁₆H₂₄INO₅

Molecular Weight: 437.274

Accurate Mass: 437.069922

Percentage Composition: C 43.95%; H 5.53%; I 29.02%; N 3.20%; O 18.29%

Melting Point: Mp 185-186° (178-179°)

>>Derivative: Sulfate

CAS Registry Number: 6509-38-2

Molecular Formula: C₁₆H₂₅NO₈S

Molecular Weight: 391.441

Accurate Mass: 391.130089

Percentage Composition: C 49.09%; H 6.44%; N 3.58%; O 32.70%; S 8.19%

Melting Point: Mp 186-188° (anhyd.). Mp 126.5-127.5 dec.° (dihydrate)

>>Derivative: *O*-β-D-Glucopyranoside

CAS Registry Number: 21848-40-8

Extra CAS Registry Numbers(s): 87206-57-3 87206-59-5

Molecular Formula: C₂₂H₃₄NO₁₀⁽⁺⁾

Molecular Weight: 472.511

Accurate Mass: 472.218274

Percentage Composition: C 55.92%; H 7.25%; N 2.96%; O 33.86%

Physical Description: Semicryst. (as acetate salt)

UV: [neutral] λ_{max} 315 () (H₂O)

Other Data: Obt. as a mix. of *E*- and *Z*-isomers

References:

- Gadamer, J., *Arch. Pharm. (Weinheim, Ger.)*, 1897, **235**, 44, (*isol*)
Späth, E., *Monatsh. Chem.*, 1920, **41**, 271, (*synth*)
Kung, H.P. *et al.*, *J.A.C.S.*, 1949, **71**, 1836, (*isol, uv*)
Schwartz, P., *Naturwissenschaften*, 1949, **36**, 88, (*isol*)
Tzagoloff, A., *Plant Physiol.*, 1963, **38**, 202, (*metab*)
Durkee, A.B. *et al.*, *J. Food Sci.*, 1975, **40**, 820, (*occur*)
Sosulski, F.W., *Dev. Food Proteins*, 1983, **2**, 109, (*rev*)
Larsen, L.M. *et al.*, *Phytochemistry*, 1983, **22**, 219-222, (*glucoside*)
Regenbrecht, J. *et al.*, *Phytochemistry*, 1985, **24**, 407