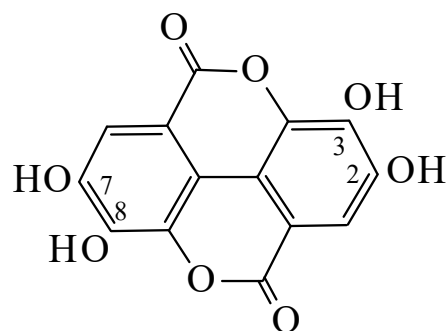




>>Entry Name: Ellagic acid, INN

ENTRY UNDER REVIEW

Synonym(s): 2,3,7,8-Tetrahydroxy[1]benzopyrano[5,4,3-*cde*][1]benzopyran-5,10-dione, 9CI. Benzoaric acid. Elagostasine. Lagistase. Alizarin yellow. Kajidin. **Gallogen**‡



CAS Registry Number: 476-66-4

Type of Compound Code(s): WK2000 WA2800 XA2500 XA4500 WK1500 XA1950 VM6100

Molecular Formula: C₁₄H₆O₈

Molecular Weight: 302.197

Accurate Mass: 302.00627

Percentage Composition: C 55.64%; H 2.00%; O 42.35%

General Statement: CAS numbering shown, other systems freq. used. Parent compd. has 2-fold symmetry with 2=7 and 3=8

Biological Source: Widely distributed in higher plants; found by Bate-Smith in 75 genera of dicotyledons and in only one monocotyledonous sp., *Hypoxis filiformis*

Biological Use/Importance: Astringent (intestinal), haemostatic, antioxidant, antineoplastic and antimutagenic agent. Dietary role *in vivo* disputed

Physical Description: Yellow needles + 2Py (Py)

Development Status: No longer marketed

Melting Point: Mp 360°

Solubility: Spar. sol. H₂O, EtOH; insol. Et₂O; sol. hot Py; BERDY SOL: Sol. MeOH, bases; fairly sol. Py; poorly sol. butanol, H₂O, hexane

Calculated Log P Data: Log P 0.26 (calc)

UV: [base] λ_{max} 257 (ε 10000); 292 (ε 20000) (EtOH/NaOH) (Derep) [neutral] λ_{max} 255 (ε 39800); 362 (ε 8510) (EtOH) (Derep) [neutral] λ_{max} 235 (ε 39800); 366 (ε 8511) (MeOH) (Berdy)

Hazard & Toxicity: Exp. reprod. effects

Fluka: 45140

Sigma: E2250

>>Derivative: Tetra-Ac

CAS Registry Number: 4274-26-4

Molecular Formula: C₂₂H₁₄O₁₂

Molecular Weight: 470.345

Accurate Mass: 470.04853

Percentage Composition: C 56.18%; H 3.00%; O 40.82%

Melting Point: Mp 317-319°. Mp 343-346°

>>Derivative: 2-*O*-Sulfate

CAS Registry Number: 124888-87-5

Type of Compound Code(s): VM6100

Molecular Formula: C₁₄H₆O₁₁S

Molecular Weight: 382.261

Accurate Mass: 381.963085

Percentage Composition: C 43.99%; H 1.58%; O 46.04%; S 8.39%

Biological Source: Constit. of *Potentilla candicans*

Biological Use/Importance: Aldose reductase inhibitor

Physical Description: Yellow needles (EtOH aq.) (as K salt)

Melting Point: Mp 297-298 dec.° (K salt)

>>Derivative: 2-*O*-β-D-Xylopyranoside

CAS Registry Number: 139163-18-1

Type of Compound Code(s): VM6100

Molecular Formula: C₁₉H₁₄O₁₂

Molecular Weight: 434.312

Accurate Mass: 434.04853

Percentage Composition: C 52.54%; H 3.25%; O 44.21%

Biological Source: Isol. from *Agrimonia pilosa* and *Platycarya strobilacea*

Physical Description: Tan powder

Melting Point: Mp 253-255 dec.°

Optical Rotation: [α]