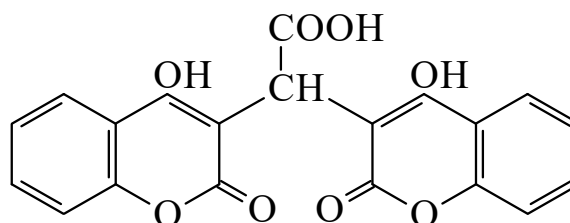




>>Entry Name: Bis[4-hydroxy-2-oxo-2H-1-benzopyran-3-yl]acetic acid, 9CI

Synonym(s): Bis(4-hydroxy-3-coumarinyl)acetic acid. Carboxymethylenebis-4-hydroxycoumarin. Pelentanic acid



CAS Registry Number: 567-83-9

Molecular Formula: C₂₀H₁₂O₈

Molecular Weight: 380.31

Accurate Mass: 380.05322

Percentage Composition: C 63.16%; H 3.18%; O 33.66%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 244-245°

>>Derivative: Me ester

Molecular Formula: C₂₁H₁₄O₈

Molecular Weight: 394.337

Accurate Mass: 394.06887

Percentage Composition: C 63.96%; H 3.58%; O 32.46%

Physical Description: Needles (AcOH)

Melting Point: Mp 202-204°

>>Derivative: Et ester

Synonym(s): Ethyl biscoumacetate, BAN, INN. Dicumacyl. Ethyl dicoumarol. Tromexan. Many other names

CAS Registry Number: 548-00-5

Molecular Formula: C₂₂H₁₆O₈

Molecular Weight: 408.364

Accurate Mass: 408.08452

Percentage Composition: C 64.71%; H 3.95%; O 31.34%

Use/Importance: Powerful orally active anticoagulant

Physical Description: Amorph. or cryst. (Me₂CO)

Melting Point: Mp 151° (amorph.). Mp 173° (cryst.)

Calculated Log P Data: Log P 3.21 (calc)

Hazard & Toxicity: Human teratogen. LD₅₀ (rat, orl) 840 mg/kg

References:

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