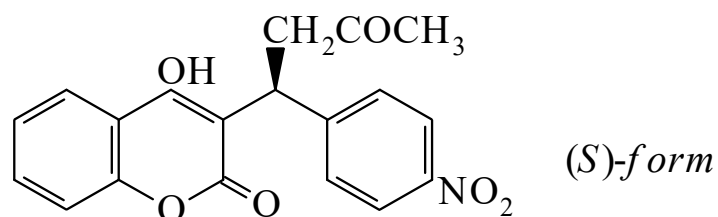




>>Entry Name: **Acenocoumarol**, INN

Synonym(s): 4-Hydroxy-3-[1-(4-nitrophenyl)-3-oxobutyl]-2*H*-1-benzopyran-2-one, 9CI. 3-(α -Acetonyl-4-nitrobenzyl)-4-hydroxycoumarin, 8CI. 3-(2-Acetyl-1-*p*-nitrophenylethyl)-4-hydroxycoumarin. **Nicoumalone**, BAN. Acenocoumarin. Sinthrome. Sintrom. G 23350. Many other names



CAS Registry Number: 152-72-7

Molecular Formula: C₁₉H₁₅NO₆

Molecular Weight: 353.331

Accurate Mass: 353.089939

Percentage Composition: C 64.59%; H 4.28%; N 3.96%; O 27.17%

Use/Importance: Oral anticoagulant

Calculated Log P Data: Log P 2.68 (calc)

Hazard & Toxicity: Human teratogenic effects. LD₅₀ (rat, orl) 513 mg/kg

>>Variant: (*R*)-form

CAS Registry Number: 66556-77-2

Molecular Formula: C₁₉H₁₅NO₆

Molecular Weight: 353.331

Accurate Mass: 353.089939

Percentage Composition: C 64.59%; H 4.28%; N 3.96%; O 27.17%

Other Data: Pharmacol. active isomer

>>Variant: (*S*)-form

CAS Registry Number: 66556-78-3

Molecular Formula: C₁₉H₁₅NO₆

Molecular Weight: 353.331

Accurate Mass: 353.089939

Percentage Composition: C 64.59%; H 4.28%; N 3.96%; O 27.17%

Melting Point: Mp 191-192°

Optical Rotation: [α]_D -225 (c, 1 in 0.5*M* NaOH)

>>Variant: ($\pm$)-form

CAS Registry Number: 70897-81-3

Molecular Formula: C₁₉H₁₅NO₆

Molecular Weight: 353.331

Accurate Mass: 353.089939

Percentage Composition: C 64.59%; H 4.28%; N 3.96%; O 27.17%

Physical Description: Cryst. (Me₂CO aq.)

Melting Point: Mp 196-199°

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