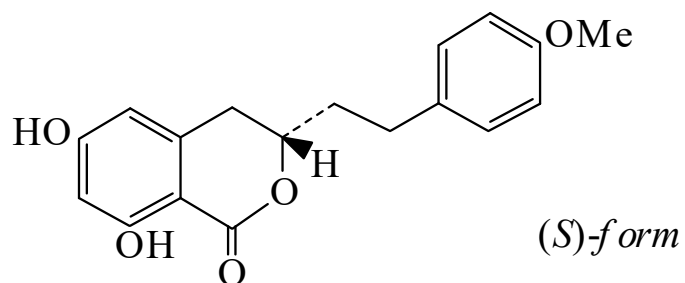




>>Entry Name: Agrimonolide

Synonym(s): 3,4-Dihydro-6,8-dihydroxy-3-[2-(4-methoxyphenyl)ethyl]-1*H*-2-benzopyran-1-one, 9Cl. 3,4-Dihydro-6,8-dihydroxy-3-(*p*-methoxyphenethyl)isocoumarin, 8Cl



Molecular Formula: C₁₈H₁₈O₅

Molecular Weight: 314.337

Accurate Mass: 314.115425

Percentage Composition: C 68.78%; H 5.77%; O 25.45%

Biological Use/Importance: Anthelmintic

Calculated Log P Data: Log P 3.85 (calc)

>>Variant: (*S*)-form

CAS Registry Number: 21499-24-1

Molecular Formula: C₁₈H₁₈O₅

Molecular Weight: 314.337

Accurate Mass: 314.115425

Percentage Composition: C 68.78%; H 5.77%; O 25.45%

Biological Source: Obt. from rhizome of *Agrimonia pilosa*

Physical Description: Columns (MeOH)

Melting Point: Mp 175.5-176.5°

Optical Rotation: [α]_D¹⁸+8.1 (c, 3.22 in Me₂CO)

Other Data: Pharmacol. active isomer

>>Derivative: 6-*O*-β-D-Glucopyranoside

Synonym(s): 6-*O*-β-D-Glucopyranosylagrimonolide

CAS Registry Number: 126223-29-8

Molecular Formula: C₂₄H₂₈O₁₀

Molecular Weight: 476.479

Accurate Mass: 476.16825

Percentage Composition: C 60.50%; H 5.92%; O 33.58%

Biological Source: Constit. of *Agrimonia pilosa*. Component of Xian He Cao

Physical Description: Cryst.

Melting Point: Mp 165-167°

Optical Rotation: [α]_D¹⁴-30.8 (c, 1 in Me₂CO)

>>Derivative: Di-Me ether

Molecular Formula: C₂₀H₂₂O₅

Molecular Weight: 342.391

Percentage Composition: C 70.16%; H 6.48%; O 23.36%

Physical Description: Needles (MeOH)

Melting Point: Mp 104-106°

>>Variant: (±)-form

CAS Registry Number: 59367-56-5

Molecular Formula: C₁₈H₁₈O₅

Molecular Weight: 314.337

Accurate Mass: 314.115425

Percentage Composition: C 68.78%; H 5.77%; O 25.45%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 173-174°

References: