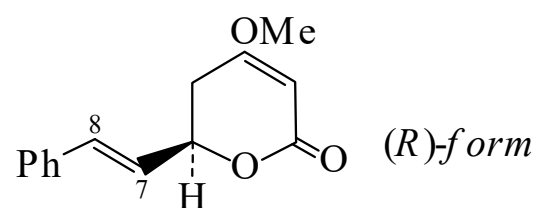




>>Entry Name: Kawain

Synonym(s): 5,6-Dihydro-4-methoxy-6-(2-phenylethenyl)-2*H*-pyran-2-one, 9Cl. Kavain



Related CAS Registry Numbers(s): 19451-52-6 19902-90-0 24576-85-0 73536-68-2

Molecular Formula: C₁₄H₁₄O₃

Molecular Weight: 230.263

Accurate Mass: 230.094295

Percentage Composition: C 73.03%; H 6.13%; O 20.84%

Use/Importance: Anaesthetic. Antiinflammatory, antipyretic agent. Shows muscle relaxant props.

Calculated Log P Data: Log P 1.85 (calc)

>>Variant: (*R*)-form

CAS Registry Number: 500-64-1

Molecular Formula: C₁₄H₁₄O₃

Molecular Weight: 230.263

Accurate Mass: 230.094295

Percentage Composition: C 73.03%; H 6.13%; O 20.84%

Biological Source: Occurs in the roots of *Piper methysticum*

Physical Description: Prisms (Et₂O/MeOH)

Melting Point: Mp 106° (110°)

Boiling Point: Bp_{0.1} 195-197°

Optical Rotation: [α]_D²⁰+105 (EtOH)

Solubility: BERDY SOL: Sol. MeOH, Et₂O; fairly sol. hexane; poorly sol. H₂O

UV: [neutral] λ_{max} 245 (ε 25500) (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, orl) 1130 mg/kg

>>Derivative: 7,8-Dihydro

Synonym(s): Marindinin. Dihydrokawain

CAS Registry Number: 587-63-3

Molecular Formula: C₁₄H₁₆O₃

Molecular Weight: 232.279

Accurate Mass: 232.109945

Percentage Composition: C 72.39%; H 6.94%; O 20.66%

Biological Source: Isol. from Kawa root (*Piper methysticum*) and *Aniba gigantica*

Use/Importance: Anaesthetic, antiinflammatory, antipyretic agent. Shows muscle relaxant props.

Physical Description: Prisms (Et₂O/petrol)

Melting Point: Mp 56-60°

Optical Rotation: [α]_D¹⁹+30 (EtOH)

Calculated Log P Data: Log P 2.15 (calc)

Other Data: Has (*S*)-config. (change of Cahn-Ingold-Prelog priorities)

Hazard & Toxicity: LD₅₀ (mus, orl) 920 mg/kg

>>Variant: (±)-form

CAS Registry Number: 3155-48-4

Molecular Formula: C₁₄H₁₄O₃

Molecular Weight: 230.263

Accurate Mass: 230.094295

Percentage Composition: C 73.03%; H 6.13%; O 20.84%

Physical Description: Cryst. (EtOAc/petrol, THF or Et₂O/MeOH)

Melting Point: Mp 146-147°

>>Derivative: 7,8-Dihydro