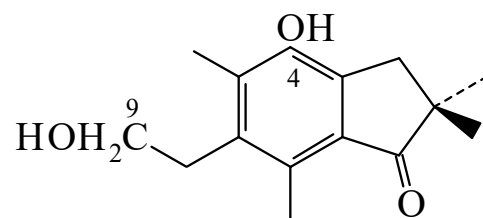




>>Entry Name: Onitin

Synonym(s): 2,3-Dihydro-4-hydroxy-6-(2-hydroxyethyl)-2,2,5,7-tetramethyl-1*H*-inden-1-one, 9Cl



CAS Registry Number: 53823-02-2

Molecular Formula: C₁₅H₂₀O₃

Molecular Weight: 248.321

Accurate Mass: 248.141245

Percentage Composition: C 72.55%; H 8.12%; O 19.33%

Biological Source: Isol. from *Onychium auratum*, *Onychium siliculosum*, *Equisetum arvense*, *Cibotium barometz* and *Dicksonia gigantea*

Use/Importance: Smooth muscle relaxant

Physical Description: Cryst. (MeOH)

Melting Point: Mp 212-214°

Calculated Log P Data: Log P 2.42 (calc)

>>Derivative: 9-*O*-β-D-Glucopyranoside

Molecular Formula: C₂₁H₃₀O₈

Molecular Weight: 410.463

Accurate Mass: 410.19407

Percentage Composition: C 61.45%; H 7.37%; O 31.18%

Biological Source: Isol. from *Cibotium barometz*

Melting Point: Mp 178-180°

Optical Rotation: [α]_D -17.7

>>Derivative: 9-*O*-β-D-Allopyranoside

Molecular Formula: C₂₁H₃₀O₈

Molecular Weight: 410.463

Accurate Mass: 410.19407

Percentage Composition: C 61.45%; H 7.37%; O 31.18%

Biological Source: Isol. from *Cibotium barometz*

Physical Description: Amorph.

Optical Rotation: [α]_D -24.8

>>Derivative: 4-*O*-β-D-Glucopyranoside

Synonym(s): Onitinoside

CAS Registry Number: 78415-48-2

Molecular Formula: C₂₁H₃₀O₈

Molecular Weight: 410.463

Accurate Mass: 410.19407

Percentage Composition: C 61.45%; H 7.37%; O 31.18%

Biological Source: Isol. from *Onychium siliculosum*

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 172-174°

>>Derivative: 9-Deoxy, 9-chloro

Synonym(s): Pterosin R

CAS Registry Number: 76947-56-3

Molecular Formula: C₁₅H₁₉ClO₂

Molecular Weight: 266.767

Accurate Mass: 266.107357

Percentage Composition: C 67.54%; H 7.18%; Cl 13.29%; O 12.00%

Biological Source: Isol. from *Cibotium barometz*

Melting Point: Mp 199.5-200°