



CAS Registry Number: 74148-51-9

Molecular Formula: C₂₅H₃₆O₉

Molecular Weight: 480.554

Accurate Mass: 480.235935

Percentage Composition: C 62.49%; H 7.55%; O 29.96%

Biological Source: Isol. from *Ailanthus excelsa*

Physical Description: Cryst. (MeOH)

Melting Point: Mp 268-270°

>> **Derivative:** 15-(2-Hydroxy-2-methylbutanoyl)

Synonym(s): Glaucarubin, β-Kirondrin

CAS Registry Number: 1448-23-3

Molecular Formula: C₂₅H₃₆O₁₀

Molecular Weight: 496.553

Accurate Mass: 496.23085

Percentage Composition: C 60.47%; H 7.31%; O 32.22%

Biological Source: Isol. from *Simarouba glauca* and *Perriera madagascariensis*

Use/Importance: Antiamoebic agent

Physical Description: Cryst.

Melting Point: Mp 250-255 dec.°

Optical Rotation: [α]_D²⁵ +69 (c, 0.6 in MeOH)

Calculated Log P Data: Log P -2.3 (uncertain value) (calc)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (rats, orl) 800 mg/kg , LD₅₀ (mus, scu) 28 mg/kg

>> **Derivative:** 15-(2-Acetoxy-2-methylbutanoyl)

Synonym(s): 2'-Acetylglaucarubin

CAS Registry Number: 68703-93-5

Molecular Formula: C₂₇H₃₈O₁₁

Molecular Weight: 538.591

Accurate Mass: 538.241415

Percentage Composition: C 60.21%; H 7.11%; O 32.68%

Biological Source: Constit. of *Simarouba amara*

Physical Description: Cryst.

Melting Point: Mp 243-246°

Optical Rotation: [α]_D +29.5 (c, 1.1 in Py)

Solubility: BERDY SOL: Sol. MeOH, CHCl₃; poorly sol. H₂O

UV: [neutral] $\lambda_{\max}$ 240 (ϵ 10700) (EtOH) (Berdy)

>> **Derivative:** 2-Ketone

Synonym(s): Glaucarubolone

CAS Registry Number: 1990-01-8

Molecular Formula: C₂₀H₂₆O₈

Molecular Weight: 394.421

Accurate Mass: 394.16277

Percentage Composition: C 60.90%; H 6.64%; O 32.45%

Biological Source: Constit. of *Hannoa klaineana* and *Castela nicholsoni*

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 255-258°

Optical Rotation: [α]_D -34 (c, 1.5 in Py)

UV: [neutral] $\lambda_{\max}$ 240 (ϵ 9000) (EtOH) (Berdy)