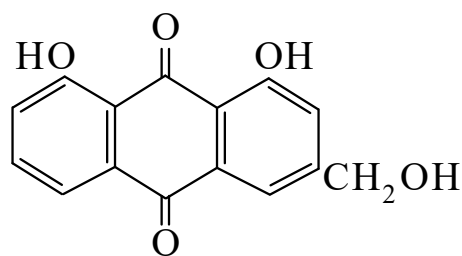




>>Entry Name: 1,8-Dihydroxy-3-hydroxymethylantraquinone, 8Cl

ENTRY UNDER REVIEW

Synonym(s): 1,8-Dihydroxy-3-hydroxymethyl-9,10-anthracenedione, 9Cl. 3-(Hydroxymethyl)chrysazin. **Aloe emodin**. **Rottlerin**‡



CAS Registry Number: 481-72-1

Molecular Formula: C₁₅H₁₀O₅

Molecular Weight: 270.241

Accurate Mass: 270.052825

Percentage Composition: C 66.67%; H 3.73%; O 29.60%

Biological Source: Found in aloes, also bark of cascara sagrada *Rhamnus purshiana*, *Rhamnus alaternus*, Chinese rhubarb *Rheum palmatum* and *Rheum undulatum*; *Rumex orientalis* and leaf fruit of *Cassia alata*. Also from *Asphodelus microcarpus*, *Asphodelus fistulosus*, *Xanthorrhoea australis* and *Oroxylum indicum*

Use/Importance: Shows some antileukaemic activity. Starting material for synth. of anthracycline antibiotics. Cathartic agent, antiseptic agent

Physical Description: Orange needles (toluene)

Melting Point: Mp 221-223°

pKa Value: pK_a 10.17 (25°, H₂O)

Calculated Log P Data: Log P 0.88 (calc)

Sigma: A7687

>>Derivative: 1'-Ac

Synonym(s): 3-(Acetoxymethyl)-1,8-dihydroxyanthraquinone. **Aloe emodin ω-acetate**

CAS Registry Number: 65615-58-9

Molecular Formula: C₁₇H₁₂O₆

Molecular Weight: 312.278

Accurate Mass: 312.06339

Percentage Composition: C 65.39%; H 3.87%; O 30.74%

Biological Source: Isol. from roots of *Rumex acetosa*, and leaves of *Kniphofia foliosa*

Physical Description: Yellow granules (C₆H₆/petrol)

Melting Point: Mp 213-214°

>>Derivative: Tri-Ac

Physical Description: Yellow needles (C₆H₆)

Melting Point: Mp 177-178°

>>Derivative: Tribenzoyl

Melting Point: Mp 234-235°

>>Derivative: 8-β-D-Glucoside

CAS Registry Number: 33037-46-6

Molecular Formula: C₂₁H₂₀O₁₀

Molecular Weight: 432.383

Accurate Mass: 432.10565

Percentage Composition: C 58.34%; H 4.66%; O 37.00%

Biological Source: Found in Chinese rhubarb (*Rheum palmatum*), cascara sagrada (*Rhamnus purshiana*) and Alexandria senna (*Cassia acutifolia*)

Physical Description: Yellow needles + ½ H₂O (CHCl₃)

Melting Point: Mp 237-238°