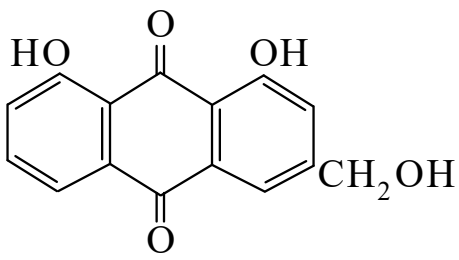
>>**Entry Name: 1,8-Dihydroxy-3-hydroxymethylanthraquinone,** 8CI
ENTRY UNDER REVIEW
Synonym(s): 1,8-Dihydroxy-3-hydroxymethyl-9,10-anthracenedione, 9CI. 3-(Hydroxymethyl)chrysazin. **Aloe emodin. Rottlerin‡**



CAS Registry Number: 481-72-1

Molecular Formula: $C_{15}H_{10}O_5$
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°, H_2O)
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: $C_{17}H_{12}O_6$
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 (C_6H_6/petrol)
Melting Point: Mp 213-214°

>>**Derivative:** Tri-Ac

Physical Description: Yellow needles (C_6H_6)
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: $C_{21}H_{20}O_{10}$
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 H_2O ($CHCl_3$)
Melting Point: Mp 237-238°

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