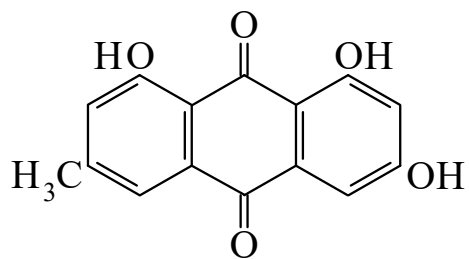




>>Entry Name: 1,3,8-Trihydroxy-6-methylanthraquinone, 8Cl

ENTRY UNDER REVIEW

Synonym(s): 1,3,8-Trihydroxy-6-methyl-9,10-anthracenedione, 9Cl. **Emodin**. Rheum-emodin. Frangula emodin. Archin. Frangulinic acid. Emodol. Alatinone



CAS Registry Number: 518-82-1

Molecular Formula: C₁₅H₁₀O₅

Molecular Weight: 270.241

Accurate Mass: 270.052825

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

Biological Source: Present in Cascara sagrada, in aloes and in other plant material. Isol. from *Penicillium* spp., *Aspergillus* spp. and from *Anixiella micropetrusa*

Biological Use/Importance: Antimicrobial, antineoplastic agent. Cathartic agent. Shows monoamine oxidase inhibitory activity

Physical Description: Orange or yellow-brown needles (Py aq. or MeOH)

Melting Point: Mp 266-268° (264-265°)

Calculated Log P Data: Log P 1.8 (calc)

UV: [acid] λ_{max} 222 (ε 35500); 252 (ε 18200); 265 (ε 18600); 289 (ε 21900); 437 (ε 12600) (EtOH) (Derep)

Hazard & Toxicity: LD₅₀ (mus, ipr) 35 mg/kg

Aldrich: 23051-0

Fluka: 45170

Sigma: E7881

>>Derivative: 3-*O*-β-D-Apiofuranoside

Synonym(s): Frangulin B

CAS Registry Number: 14101-04-3

Molecular Formula: C₂₀H₁₈O₉

Molecular Weight: 402.357

Accurate Mass: 402.095085

Percentage Composition: C 59.70%; H 4.51%; O 35.79%

Biological Source: From *Rhamnus frangula*

Melting Point: Mp 196°

>>Derivative: 3-*O*-β-D-Apiofuranoside, 1-*O*-β-D-glucopyranoside

Synonym(s): Glucofrangulin B

CAS Registry Number: 14062-59-0

Molecular Formula: C₂₆H₂₈O₁₄

Molecular Weight: 564.499

Accurate Mass: 564.14791

Percentage Composition: C 55.32%; H 5.00%; O 39.68%

Biological Source: From *Rhamnus frangula*

Other Data: Probable struct.

>>Derivative: 1-*O*-α-L-Arabinopyranoside

CAS Registry Number: 82780-62-9

Molecular Formula: C₂₀H₁₈O₉

Molecular Weight: 402.357

Accurate Mass: 402.095085

Percentage Composition: C 59.70%; H 4.51%; O 35.79%

Physical Description: Yellow cryst.

Melting Point: Mp 162°