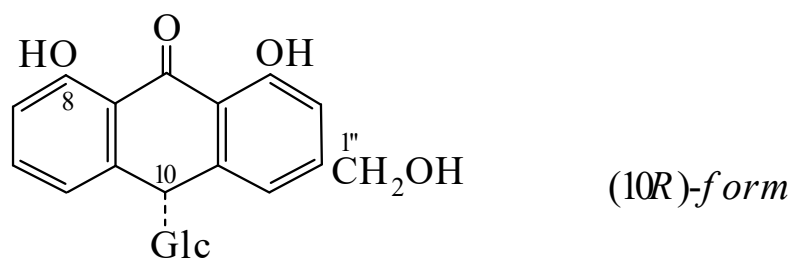




>>Entry Name: Aloin, BAN

ENTRY UNDER REVIEW

Synonym(s): 10-β-D-Glucopyranosyl-1,8-dihydroxy-3-(hydroxymethyl)-9(10*H*)-anthracenone, 9Cl. Barbaloin. Socaloin. Ugandaloin. Jafaloin. Cafaloin



CAS Registry Number: 8015-61-0

Related CAS Registry Numbers(s): 5133-19-7 73889-54-0 138373-24-7

Molecular Formula: C₂₁H₂₂O₉

Molecular Weight: 418.399

Accurate Mass: 418.126385

Percentage Composition: C 60.28%; H 5.30%; O 34.42%

General Statement: Aloin as normally obt. is a mixt. of 10-epimers separable by hplc into Aloin A and the unstable Aloin B. Aloin A can also be obt. by cryst. from MeOH

Biological Source: Constit. of various *Aloe* spp.

Use/Importance: Purgative, laxative

Solubility: BERDY SOL: Sol. H₂O

Calculated Log P Data: Log P -1.88 (calc)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ivn) 200 mg/kg

>>Variant: (10*R*)-form

Synonym(s): Aloin B. Isobarbaloin. β-Barbaloin

CAS Registry Number: 28371-16-6

Molecular Formula: C₂₁H₂₂O₉

Molecular Weight: 418.399

Accurate Mass: 418.126385

Percentage Composition: C 60.28%; H 5.30%; O 34.42%

Melting Point: Mp 138-140° (block)

Optical Rotation: [α]_D³⁰ -73 (c, 0.5 in MeOH)

Other Data: Negative CD at 295 nm. Pmr δ 5.27 (C-1'). Labile in soln. Isobarbaloin and β-Barbaloin were prob. not homogeneous

>>Derivative: 8-*O*-β-D-Glucopyranoside

Synonym(s): Cascaroside B

CAS Registry Number: 53861-34-0

Molecular Formula: C₂₇H₃₂O₁₄

Molecular Weight: 580.541

Accurate Mass: 580.17921

Percentage Composition: C 55.86%; H 5.56%; O 38.58%

Biological Source: Isol. from *Rhamnus purshiana* (Cascara sagrada) bark

Physical Description: Cryst. + 2H₂O

Melting Point: Mp 175-178°

Optical Rotation: [α]_D³⁰ -104.4 (MeOH)

Other Data: See remark above about stereochem

>>Derivative: 1''-*O*-α-L-Rhamnopyranoside

Synonym(s): Aloinoside B

CAS Registry Number: 11006-91-0

Molecular Formula: C₂₇H₃₂O₁₃

Molecular Weight: 564.542

Accurate Mass: 564.184295

Percentage Composition: C 57.44%; H 5.71%; O 36.84%

Biological Source: Isol. from leaves of *Aloe* cf. *perryi*

Physical Description: Cryst. (Me₂CO aq.)

Melting Point: Mp 233°

Optical Rotation: [α]_D²⁰ -45.3 (c, 1.5 in 50% dioxan aq.)