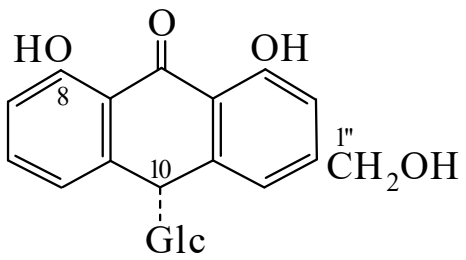
>>**Entry Name: Aloin,** BAN
ENTRY UNDER REVIEW
Synonym(s): 10-β-D-Glucopyranosyl-1,8-dihydroxy-3-(hydroxymethyl)-9(10*H*)-anthracenone, 9CI. Barbaloin. Socaloin. Ugandaloin. Jafaloin. Cafaloin



(10*R*)-*form*

CAS Registry Number: 8015-61-0
Related CAS Registry Numbers(s): 5133-19-7 73889-54-0 138373-24-7

Molecular Formula: $C_{21}H_{22}O_9$
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. H_2O
Calculated Log P Data: Log P –1.88 (calc)
Hazard & Toxicity: BERDY HAZD : LD_{50} (mus, ivn) 200 mg/kg

>>**Variant:** (10*R*)-form
Synonym(s): Aloin B. Isobarbaloin. β-Barbaloin

CAS Registry Number: 28371-16-6

Molecular Formula: $C_{21}H_{22}O_9$
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: $[\alpha]_D^{30}$ –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: $C_{27}H_{32}O_{14}$
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. + $2H_2O$
Melting Point: Mp 175-178°
Optical Rotation: $[\alpha]_D^{30}$ –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: $C_{27}H_{32}O_{13}$
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. (Me_2CO aq.)
Melting Point: Mp 233°
Optical Rotation: $[\alpha]_D^{20}$ –45.3 (c, 1.5 in 50% dioxan aq.)