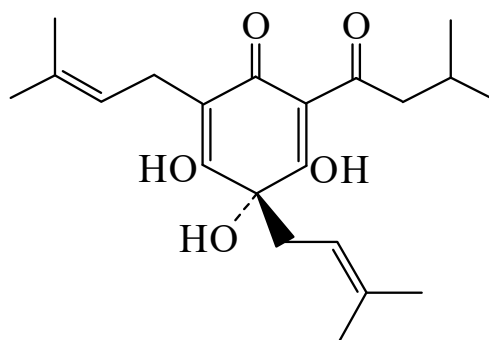




>>Entry Name: Humulone

Synonym(s): α -Lupulinic acid. α -Bitter acid. α -Lupulic acid



CAS Registry Number: 26472-41-3

Molecular Formula: $C_{21}H_{30}O_5$

Molecular Weight: 362.465

Accurate Mass: 362.209325

Percentage Composition: C 69.59%; H 8.34%; O 22.07%

Use/Importance: Antispasmodic agent. Active against gram-positive bacteria

Calculated Log P Data: Log P 3.88 (calc)

>>Variant: (*R*)-form

Molecular Formula: $C_{21}H_{30}O_5$

Molecular Weight: 362.465

Accurate Mass: 362.209325

Percentage Composition: C 69.59%; H 8.34%; O 22.07%

Biological Source: Constit. of hops

Physical Description: Cryst.

Melting Point: Mp 66-66.5°

Optical Rotation: $[\alpha]_D^{20} -232.2$

Solubility: BERDY SOL: Sol. MeOH, hexane; fairly sol. acids; poorly sol. H_2O

UV: [neutral] λ_{max} 236 (E1%/1cm 390); 283 (); 323 () (MeOH) (Berdy) [acid] λ_{max} 235 (ϵ 10100); 281 (ϵ 8000); 320 (ϵ 5330) (EtOH-HCl) (Berdy) [base] λ_{max} 228 (ϵ 14700); 324 (ϵ 11000); 368 (ϵ 8700) (EtOH-NaOH) (Berdy)

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