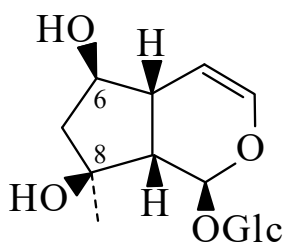




>>Entry Name: Ajugol

Synonym(s): Leonuride



CAS Registry Number: 52949-83-4

Molecular Formula: C₁₅H₂₄O₉

Molecular Weight: 348.349

Accurate Mass: 348.142035

Percentage Composition: C 51.72%; H 6.94%; O 41.34%

Biological Source: Constit. of *Ajuga reptans*, *Melittis melissophyllum*, *Rehmannia glutinosa* and *Leonurus cardiaca*

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_{\text{D}}^{24} -172.1$ (c, 0.53 in MeOH)

>>Derivative: 6-Ac

Synonym(s): 6-Acetylajugol

Molecular Formula: C₁₇H₂₆O₁₀

Molecular Weight: 390.386

Accurate Mass: 390.1526

Percentage Composition: C 52.30%; H 6.71%; O 40.98%

Biological Source: Constit. of *Leonurus persicus*

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_{\text{D}}^{20} -103.5$ (c, 0.07 in MeOH)

UV: [neutral] λ_{max} 210 (log ϵ 4.32); 232 (log ϵ 4.31) (MeOH)

>>Derivative: 8-Ac

Synonym(s): Ajugoside

CAS Registry Number: 52916-96-8

Molecular Formula: C₁₇H₂₆O₁₀

Molecular Weight: 390.386

Accurate Mass: 390.1526

Percentage Composition: C 52.30%; H 6.71%; O 40.98%

Biological Source: Constit. of *Ajuga reptans*, *Melittis melissophyllum* and *Leonurus cardiaca*

Physical Description: Amorph. powder

UV: [neutral] λ_{max} 206 () (MeOH) (Berdy)

>>Derivative: Hexa-Ac

CAS Registry Number: 50515-38-3

Molecular Formula: C₂₇H₃₆O₁₅

Molecular Weight: 600.572

Accurate Mass: 600.205425

Percentage Composition: C 54.00%; H 6.04%; O 39.96%

Melting Point: Mp 174-175°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -200$ (c, 2 in CHCl₃)

>>Derivative: 6-O-(4-Hydroxybenzoyl)

Synonym(s): 6-O-(4-Hydroxybenzoyl)ajugol

CAS Registry Number: 125180-69-0

Molecular Formula: C₂₂H₂₈O₁₁

Molecular Weight: 468.457

Accurate Mass: 468.163165

Percentage Composition: C 56.41%; H 6.02%; O 37.57%

Biological Source: Constit. of *Rehmannia glutinosa* and *Tabebuia avellanedae*

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_{\text{D}}^{29} -138.8$ (c, 0.1 in MeOH)