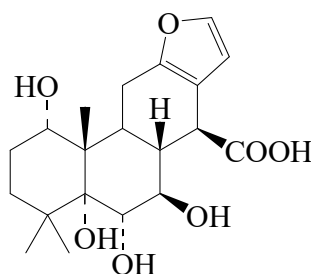




>>Entry Name: 1,5,6,7-Tetrahydroxy-17-vouacapanoic acid



Molecular Formula: C₂₀H₂₈O₇

Molecular Weight: 380.437

Accurate Mass: 380.183505

Percentage Composition: C 63.14%; H 7.42%; O 29.44%

>>Variant: (1 α ,6 α ,7 β)-form

Molecular Formula: C₂₀H₂₈O₇

Molecular Weight: 380.437

Accurate Mass: 380.183505

Percentage Composition: C 63.14%; H 7.42%; O 29.44%

>>Derivative: 1,6-Di-Ac, Me ester

Synonym(s): Bonducellpin A

CAS Registry Number: 197781-82-1

Molecular Formula: C₂₅H₃₄O₉

Molecular Weight: 478.538

Accurate Mass: 478.220285

Percentage Composition: C 62.75%; H 7.16%; O 30.09%

Biological Source: Constit. of *Caesalpinia bonduc*

Physical Description: Cryst.

Melting Point: Mp 118-119°

Optical Rotation: [α]_D +4.6 (c, 0.33 in CHCl₃)

UV: [neutral] $\lambda_{\max}$ 226 (log ϵ 3.76) (MeOH)

>>Derivative: 1-Ketone, 6-Ac, Me ester

Synonym(s): Bonducellpin B

CAS Registry Number: 197781-83-2

Molecular Formula: C₂₃H₃₀O₈

Molecular Weight: 434.485

Accurate Mass: 434.19407

Percentage Composition: C 63.58%; H 6.96%; O 29.46%

Biological Source: Constit. of *Caesalpinia bonduc*

Physical Description: Gum

Optical Rotation: [α]_D +18.7 (c, 0.14 in CHCl₃)

UV: [neutral] $\lambda_{\max}$ 218 (log ϵ 3.74); 254 (log ϵ 3.29) (MeOH)

>>Derivative: 17 $\rightarrow$ 7 Lactone, 6-Ac

Synonym(s): Bonducellpin D

CAS Registry Number: 197781-85-4

Molecular Formula: C₂₂H₂₈O₇

Molecular Weight: 404.459

Accurate Mass: 404.183505

Percentage Composition: C 65.33%; H 6.98%; O 27.69%

Biological Source: Constit. of *Caesalpinia bonduc*

Physical Description: Cryst.

Melting Point: Mp 216-217°

Optical Rotation: [α]_D +8.4 (c, 0.35 in CHCl₃)

UV: [neutral] $\lambda_{\max}$ 218 (log ϵ 3.84); 260 (log ϵ 3.21) (MeOH)

References:

Peter, S.R. *et al.*, *J. Nat. Prod.*, 1997, **60**, 1219-1221, (*isol*, *pmr*, *cmr*)