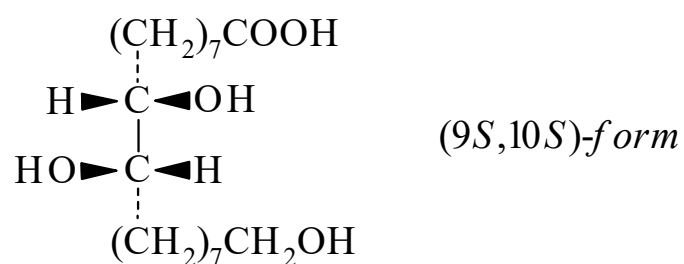




>>Entry Name: 9,10,18-Trihydroxyoctadecanoic acid
ENTRY UNDER REVIEW



CAS Registry Number: 496-86-6

Molecular Formula: C₁₈H₃₆O₅

Molecular Weight: 332.479

Accurate Mass: 332.256275

Percentage Composition: C 65.03%; H 10.91%; O 24.06%

>>Variant: (9S,10S)-form

Synonym(s): Phloionolic acid. Floionolic acid

CAS Registry Number: 17705-68-9

Molecular Formula: C₁₈H₃₆O₅

Molecular Weight: 332.479

Accurate Mass: 332.256275

Percentage Composition: C 65.03%; H 10.91%; O 24.06%

Biological Source: Constit. of cork and other plants, eg. olive (*Olea europaea*), *Agave americana*, *Chamaepeuce afra*, *Ligustrum japonicum*, apple wax and also cutins

Physical Description: Cryst. (MeOH)

Melting Point: Mp 104-105°

Optical Rotation: [α]_D +22.75

pKa Value: pK_{a1} 4.95

Other Data: The (9R,10R)-(-) form has also been prepared

>>Derivative: Me ester

CAS Registry Number: 36693-05-7

Molecular Formula: C₁₉H₃₈O₅

Molecular Weight: 346.506

Accurate Mass: 346.271925

Percentage Composition: C 65.86%; H 11.05%; O 23.09%

Melting Point: Mp 79-80.5°

Optical Rotation: [α]_D +21.52

>>Variant: (9RS,10RS)-form

Synonym(s): (±)-threo-form

CAS Registry Number: 583-86-8

Molecular Formula: C₁₈H₃₆O₅

Molecular Weight: 332.479

Accurate Mass: 332.256275

Percentage Composition: C 65.03%; H 10.91%; O 24.06%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 104°

>>Variant: (9RS,10SR)-form

Synonym(s): erythro-form. Isophloionolic acid

CAS Registry Number: 17673-81-3

Molecular Formula: C₁₈H₃₆O₅

Molecular Weight: 332.479

Accurate Mass: 332.256275

Percentage Composition: C 65.03%; H 10.91%; O 24.06%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 132-133°

Other Data: Opt. inactive (*meso*-)

References: