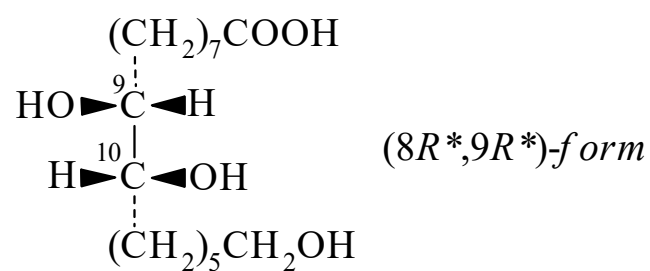




>>Entry Name: 9,10,16-Trihydroxyhexadecanoic acid

Synonym(s): 9,10,16-Trihydroxypalmitic acid



CAS Registry Number: 533-87-9

Related CAS Registry Numbers(s): 17941-34-3

Molecular Formula: C₁₆H₃₂O₅

Molecular Weight: 304.426

Accurate Mass: 304.224975

Percentage Composition: C 63.13%; H 10.59%; O 26.28%

Hazard & Toxicity: LD₅₀ (mus, ivn) 178 mg/kg

Fluka: 5540

Rare Chemicals Library: S56164-9

>>Variant: (8R*,9R*)-form

Synonym(s): (+)-threo-form

CAS Registry Number: 33447-77-7

Molecular Formula: C₁₆H₃₂O₅

Molecular Weight: 304.426

Accurate Mass: 304.224975

Percentage Composition: C 63.13%; H 10.59%; O 26.28%

Melting Point: Mp 102.5-103.5°

Optical Rotation: [α]_D +24.6

>>Derivative: Me ester

Molecular Formula: C₁₇H₃₄O₅

Molecular Weight: 318.453

Accurate Mass: 318.240625

Percentage Composition: C 64.12%; H 10.76%; O 25.12%

Melting Point: Mp 71-72°

Optical Rotation: [α]_D +23.45

>>Variant: (8S*,9S*)-form

Synonym(s): (-)-threo-form

CAS Registry Number: 33447-75-5

Molecular Formula: C₁₆H₃₂O₅

Molecular Weight: 304.426

Accurate Mass: 304.224975

Percentage Composition: C 63.13%; H 10.59%; O 26.28%

Melting Point: Mp 103-104°

Optical Rotation: [α]_D -24.45

>>Derivative: Me ester

Melting Point: Mp 72-73°

Optical Rotation: [α]_D -23.45