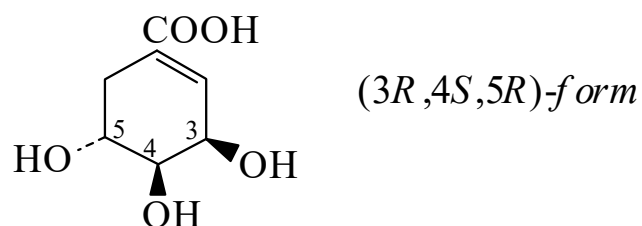




>>Entry Name: 3,4,5-Trihydroxy-1-cyclohexene-1-carboxylic acid, 9CI



CAS Registry Number: 2306-23-2

Related CAS Registry Numbers(s): 10191-00-1

Molecular Formula: C₇H₁₀O₅

Molecular Weight: 174.153

Accurate Mass: 174.052825

Percentage Composition: C 48.28%; H 5.79%; O 45.93%

that 3 becomes 5 and *vice-versa*

>>Variant: (3*R*,4*S*,5*R*)-form

Synonym(s): Shikimic acid

CAS Registry Number: 138-59-0

Molecular Formula: C₇H₁₀O₅

Molecular Weight: 174.153

Accurate Mass: 174.052825

Percentage Composition: C 48.28%; H 5.79%; O 45.93%

Biological Source: Constit. of many plants, particularly fruits of *Illicium religiosum*

Biosynthesis: Key intermediate in biosynth. of phenylalanine, phenolic cinnamates and their metabolites, e.g. flavonoids, lignans, alkaloids

Physical Description: Cryst. (H₂O)

Melting Point: Mp 178-180°. Mp 190-191°

Optical Rotation: $[\alpha]_{\text{D}}^{22} -157$ (c, 1 in H₂O)

Solubility: Insol. EtOH, Et₂O, CHCl₃

Aldrich: S320-8

Fluka: 85091

Sigma: S5375

Supelco: R47-3890

>>Derivative: MeNH₂ salt

Melting Point: Mp 163-164°

>>Derivative: Me ester

CAS Registry Number: 40983-58-2

Molecular Formula: C₈H₁₂O₅

Molecular Weight: 188.18

Accurate Mass: 188.068475

Percentage Composition: C 51.06%; H 6.43%; O 42.51%

Physical Description: Needles (AcOH/petrol)

Melting Point: Mp 113-114°

Optical Rotation: $[\alpha]_{\text{D}} -130$ (c, 1.88, EtOH)

>>Derivative: Tri-Ac

CAS Registry Number: 16613-47-1

Molecular Formula: C₁₃H₁₆O₈

Molecular Weight: 300.265

Accurate Mass: 300.08452

Percentage Composition: C 52.00%; H 5.37%; O 42.63%

Boiling Point: Bp₁ 200-210°