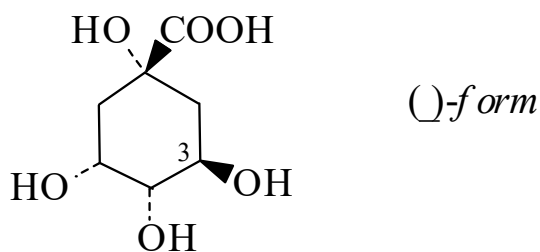




>>Entry Name: Quinic acid

ENTRY UNDER REVIEW

Synonym(s): 1,3,4,5-Tetrahydroxycyclohexanecarboxylic acid, 9CI. Hexahydro-1,3,4,5-tetrahydroxybenzoic acid. Chinic acid



CAS Registry Number: 36413-60-2

Molecular Formula:  $C_7H_{12}O_6$

Molecular Weight: 192.168

Accurate Mass: 192.06339

Percentage Composition: C 43.75%; H 6.29%; O 49.95%

>>Variant: (-)-form

CAS Registry Number: 77-95-2

Molecular Formula:  $C_7H_{12}O_6$

Molecular Weight: 192.168

Accurate Mass: 192.06339

Percentage Composition: C 43.75%; H 6.29%; O 49.95%

Biological Source: Occurs in cinchona bark, coffee beans, tobacco leaves and many other plant sources

Use/Importance: Food acidulant with good taste characteristics, use limited by cost

Melting Point: Mp 162-163°

Optical Rotation:  $[\alpha]_D^{26} -42.1$  (H<sub>2</sub>O)

Solubility: BERDY SOL: Sol. H<sub>2</sub>O

pKa Value: pK<sub>a</sub> 3.58 (25°)

UV: [neutral]  $\lambda_{max}$  (MeOH) (Berdy)

Hazard & Toxicity: LD<sub>50</sub> (mus, scu) 10000 mg/kg

Aldrich: 13862-2

Fluka: 22580

Supelco: 4-6944

>>Derivative: Lactone

Synonym(s): 1,3,4-Trihydroxy-6-oxabicyclo[3.2.1]octan-7-one, 9CI. Quinide

CAS Registry Number: 27783-00-2

Molecular Formula:  $C_7H_{10}O_5$

Molecular Weight: 174.153

Accurate Mass: 174.052825

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

Biological Source: Constit. of *Gardenia sootepensis*

Melting Point: Mp 187°

Optical Rotation:  $[\alpha]_D^{23} -16.75$  (c, 8.3 in H<sub>2</sub>O)

Other Data: Lactonised onto the C-3 OH group

>>Derivative: Tetra-Ac

Molecular Formula:  $C_{15}H_{20}O_{10}$

Molecular Weight: 360.317

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Melting Point: Mp 132-136°

Optical Rotation:  $[\alpha]_D^{20} -22.5$  (EtOH)