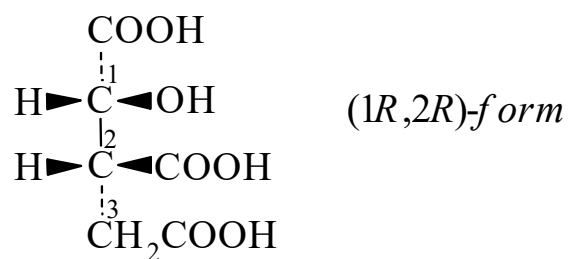




>>Entry Name: Isocitric acid

ENTRY UNDER REVIEW

Synonym(s): 1-Hydroxy-1,2,3-propanetricarboxylic acid. 1-Hydroxytricarballic acid. 3-Carboxy-3,4-dideoxypentatic acid, 9CI



CAS Registry Number: 320-77-4

Related CAS Registry Numbers(s): 1637-73-6

Molecular Formula: C₆H₈O₇

Molecular Weight: 192.125

Accurate Mass: 192.027005

Percentage Composition: C 37.51%; H 4.20%; O 58.29%

confusion in the application of the *erythro/threo* and D/L-stereodescriptors and these should be avoided

pKa Value: pK_{a1} 3.28; pK_{a2} 4.71; pK_{a3} 6.4 (25°) pK_{a1} 3.02; pK_{a2} 4.28; pK_{a3} 5.75 (25°)

>>Variant: (1*R*,2*R*)-form

Synonym(s): (–)-*erythro*-form. (–)-Alloisocitric acid

CAS Registry Number: 30810-51-6

Molecular Formula: C₆H₈O₇

Molecular Weight: 192.125

Accurate Mass: 192.027005

Percentage Composition: C 37.51%; H 4.20%; O 58.29%

Biological Source: Found in lemon juice

Optical Rotation: [α]_D –34.1 (c, 0.5-1 in H₂O)

>>Derivative: 1,4-Lactone

Synonym(s): Tetrahydro-5-oxo-2,3-furandicarboxylic acid

Molecular Formula: C₆H₆O₆

Molecular Weight: 174.11

Accurate Mass: 174.01644

Percentage Composition: C 41.39%; H 3.47%; O 55.14%

Melting Point: Mp 143°

Optical Rotation: [α]_D –40.5 (H₂O)

>>Variant: (1*R*,2*S*)-form

Synonym(s): (+)-*threo*-form. (+)-Isocitric acid

CAS Registry Number: 6061-97-8

Molecular Formula: C₆H₈O₇

Molecular Weight: 192.125

Accurate Mass: 192.027005

Percentage Composition: C 37.51%; H 4.20%; O 58.29%

Biological Source: Found in fruit juices. Produced by *Candida* spp. Occurs in blackberry and other Crassulacean plants.

Melting Point: Mp 105°

Optical Rotation: [α]_D +30.6 (H₂O)

>>Derivative: Di-Me ester

Molecular Formula: C₈H₁₂O₇

Molecular Weight: 220.179

Accurate Mass: 220.058305

Percentage Composition: C 43.64%; H 5.49%; O 50.87%

Melting Point: Mp 106°

Optical Rotation: [α]_D²⁰ –63

>>Derivative: Tri-Et ester