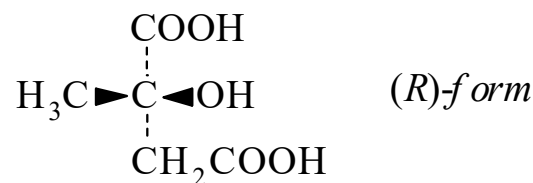




>>Entry Name: 2-Hydroxy-2-methylbutanedioic acid

ENTRY UNDER REVIEW

Synonym(s): 2-Hydroxy-2-methylsuccinic acid. Citramalic acid. 2-Methylmalic acid



CAS Registry Number: 2306-22-1

Related CAS Registry Numbers(s): 81426-68-8

Molecular Formula: C₅H₈O₅

Molecular Weight: 148.115

Accurate Mass: 148.037175

Percentage Composition: C 40.55%; H 5.44%; O 54.01%

Fluka: 27455

Rare Chemicals Library: S41537-5

>>Variant: (R)-form

CAS Registry Number: 6236-10-8

Molecular Formula: C₅H₈O₅

Molecular Weight: 148.115

Accurate Mass: 148.037175

Percentage Composition: C 40.55%; H 5.44%; O 54.01%

Biological Source: Constit. of apple peel

Optical Rotation: [α]_D −30

Other Data: Referred to as the L-form but this is ambiguous

Aldrich: 32914-2

Fluka: 27454

Sigma: C7416

>>Derivative: Di-Me ester

CAS Registry Number: 81426-68-8

Molecular Formula: C₇H₁₂O₅

Molecular Weight: 176.169

Accurate Mass: 176.068475

Percentage Composition: C 47.73%; H 6.87%; O 45.41%

Physical Description: Liq.

Boiling Point: Bp_{0.15} 90° (bath)

Optical Rotation: [α]_D²⁰ −27 (c, 1.1 in CHCl₃) (>97% ee)

>>Derivative: 1-Me ester, 4-nitrile

Synonym(s): Methyl-3-cyano-2-hydroxy-2-methylpropanoate

CAS Registry Number: 141562-85-8

Molecular Formula: C₆H₉NO₃

Molecular Weight: 143.142

Accurate Mass: 143.058244

Percentage Composition: C 50.35%; H 6.34%; N 9.79%; O 33.53%

Physical Description: Liq.

Boiling Point: Bp_{0.25} 120° (bath)

Optical Rotation: [α]_D²⁰ +8.5 (c, 1.8 in CHCl₃) (>97% ee)

>>Variant: (S)-form

CAS Registry Number: 6236-09-5

Molecular Formula: C₅H₈O₅

Molecular Weight: 148.115

Accurate Mass: 148.037175

Percentage Composition: C 40.55%; H 5.44%; O 54.01%

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 112-115°