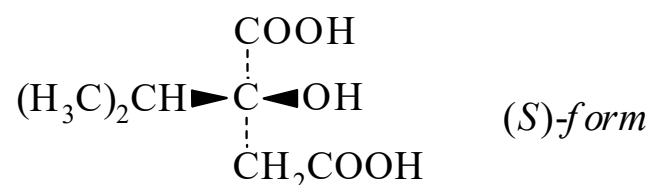




>>Entry Name: 2-Hydroxy-2-isopropylbutanedioic acid

Synonym(s): 2-Hydroxy-2-(1-methylethyl)butanedioic acid, 9CI. 2-Isopropylmalic acid, 8CI. 2-Hydroxy-2-isopropylsuccinic acid. β -Carboxy- β -hydroxyisocaproic acid



CAS Registry Number: 3237-44-3

Related CAS Registry Numbers(s): 43119-99-9 49601-06-1

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_5$

Molecular Weight: 176.169

Accurate Mass: 176.068475

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

Aldrich: 33311-5

>>Variant: (-)-form

CAS Registry Number: 49601-06-1

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_5$

Molecular Weight: 176.169

Accurate Mass: 176.068475

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

Biological Source: Prod. by various bacteria, yeast, from maize (*Zea mays*), flax (*Linum usitatissimum*) and *Sorghum vulgare*

Use/Importance: Intermed. in leucine biosynth.

Melting Point: Mp 171-173°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -20$ (c, 2.5 in MeOH)

>>Derivative: Bis(4- β -D-Glucopyranosyloxybenzyl) ester

CAS Registry Number: 90139-13-2

Molecular Formula: $\text{C}_{33}\text{H}_{44}\text{O}_{17}$

Molecular Weight: 712.7

Accurate Mass: 712.257855

Percentage Composition: C 55.61%; H 6.22%; O 38.16%

Biological Source: Constit. of *Galeola faberi* and *Galeola septentrionalis*

Physical Description: Amorph. powder (MeOH/ CHCl_3)

Melting Point: Mp 109-111°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -44.2$ (c, 1.27 in MeOH)

>>Variant: ($\pm$)-form

CAS Registry Number: 123164-17-0

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_5$

Molecular Weight: 176.169

Accurate Mass: 176.068475

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

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 145-147°

Boiling Point: Bp₁₀ 118-120°

>>Derivative: 1-Amide

Synonym(s): 2-Hydroxy-2-isopropylsuccinamic acid

Molecular Formula: $\text{C}_7\text{H}_{13}\text{NO}_4$

Molecular Weight: 175.184

Accurate Mass: 175.084459

Percentage Composition: C 47.99%; H 7.48%; N 8.00%; O 36.53%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 156-157°