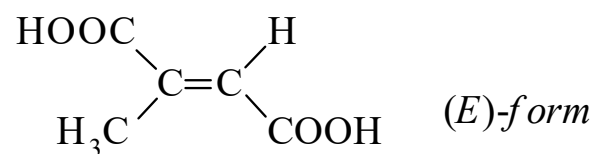




>>Entry Name: 2-Methyl-2-butenedioic acid, 9CI



CAS Registry Number: 7407-59-2

Molecular Formula: C₅H₆O₄

Molecular Weight: 130.1

Accurate Mass: 130.02661

Percentage Composition: C 46.16%; H 4.65%; O 49.19%

>>Variant: (*E*)-form

Synonym(s): Mesaconic acid, 8CI. Methylfumaric acid

CAS Registry Number: 498-24-8

Molecular Formula: C₅H₆O₄

Molecular Weight: 130.1

Accurate Mass: 130.02661

Percentage Composition: C 46.16%; H 4.65%; O 49.19%

Biological Source: Isol. from Calabash curare, found in traces in plant tissues

Physical Description: Orthorhombic needles or monoclinic tablets (EtOAc)

Melting Point: Mp 204-205°

Boiling Point: Bp 250° dec.

Solubility: Sol. EtOH, Et₂O, H₂O

pKa Value: p*K*_{a1} 3.1; p*K*_{a2} 4.83 (25°, H₂O)

Other Data: Sublimes. Mesaconic acid, and its esters, anhydride, and *N*-alkyl imines undergo radical copolym. with vinyl monomers, e.g. styrene

Aldrich: 13104-0

Fluka: 63880

Sigma: M0514

>>Derivative: 1-Mono-Me ester

Synonym(s): α-Me ester

CAS Registry Number: 39529-95-8

Molecular Formula: C₆H₈O₄

Molecular Weight: 144.127

Accurate Mass: 144.04226

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

Physical Description: Cryst. (petrol)

Melting Point: Mp 52°

Solubility: Sol. H₂O

pKa Value: p*K*_{a1} 3.45 (23°, H₂O)

>>Derivative: 4-Mono-Me ester

Synonym(s): β-Me ester

CAS Registry Number: 77044-59-8

Molecular Formula: C₆H₈O₄

Molecular Weight: 144.127

Accurate Mass: 144.04226

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

Physical Description: Needles (petrol)

Melting Point: Mp 84°

Boiling Point: Bp₁₃ 135-137°

pKa Value: p*K*_{a1} 3.29 (20°, H₂O)

>>Derivative: Di-Me ester

CAS Registry Number: 617-53-8

Molecular Formula: C₇H₁₀O₄

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Boiling Point: Bp 205.5-206.5°. Bp₁₆ 100°

Solubility: Spar. sol. H₂O; v. sol. Me₂CO, Et₂O, EtOH

Density: d