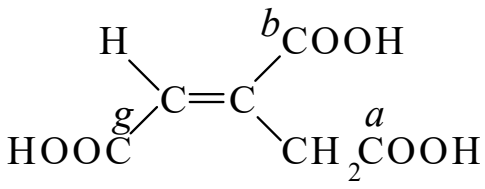
>>**Entry Name: Aconitic acid**
ENTRY UNDER REVIEW
Synonym(s): 1-Propene-1,2,3-tricarboxylic acid, 9CI. Achilleaic acid. Citridinic acid. Equisetic acid. Pyrocitric acid. 3-Carboxy-2-pentenedioic acid. FEMA 2010



(*E*)-*form*

CAS Registry Number: 499-12-7
Related CAS Registry Numbers(s): 20820-77-3 65629-33-6

Molecular Formula: $C_6H_6O_6$
Molecular Weight: 174.11
Accurate Mass: 174.01644
Percentage Composition: C 41.39%; H 3.47%; O 55.14%

Rare Chemicals Library: S43785-9

>>**Variant:** (*E*)-form

CAS Registry Number: 4023-65-8
Molecular Formula: $C_6H_6O_6$
Molecular Weight: 174.11
Accurate Mass: 174.01644
Percentage Composition: C 41.39%; H 3.47%; O 55.14%
Biological Source: Isol. from *Asarum europaeum*, from cane-sugar molasses and other plant sources. Present in large amounts in *Aconitum napellus* (monkshood)
Use/Importance: Used to prod. unsatd. polyesters. Reagent used for fluorimetric anal. of tertiary amines
Physical Description: Leaflets (H_2O)
Melting Point: Mp 194-195 dec.°
Solubility: Sol. H_2O, EtOH
pKa Value: pK_{a1} 2.8; pK_{a2} 4.46 (25°)
Other Data: Decarboxylates at Mp to Methylenebutanedioic acid HJM97-X. Mp variable with rate of htg. Several copolymers with alkenes have been synth.
Aldrich: W20100-6
Fluka: 1600
Sigma: A7376

>>**Derivative:** α-Mono-Me ester

CAS Registry Number: 65146-88-5
Molecular Formula: $C_7H_8O_6$
Molecular Weight: 188.137
Accurate Mass: 188.03209
Percentage Composition: C 44.69%; H 4.29%; O 51.02%
Physical Description: Prisms (Me_2CO/C_6H_6)
Melting Point: Mp 136-137°
Other Data: Called 3-ester in CAS

>>**Derivative:** β-Mono-Me ester

CAS Registry Number: 65146-89-6
Molecular Formula: $C_7H_8O_6$
Molecular Weight: 188.137
Accurate Mass: 188.03209
Percentage Composition: C 44.69%; H 4.29%; O 51.02%
Physical Description: Prisms (Me_2CO/C_6H_6)
Melting Point: Mp 144-145°
Other Data: Called 2-ester in CAS