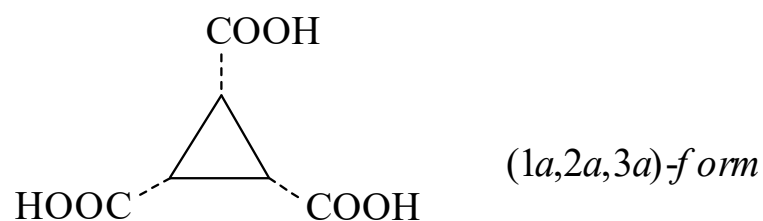




>>Entry Name: 1,2,3-Cyclopropanetricarboxylic acid, 9CI

Synonym(s): Aceconitic acid



Molecular Formula: C₆H₆O₆

Molecular Weight: 174.11

Accurate Mass: 174.01644

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

>>Variant: (1 α ,2 α ,3 α)-form

Synonym(s): *cis*-form

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 195.5-196°

pKa Value: pK_{a2} 4.5; pK_{a3} 10

>>Derivative: Tri-Me ester

Molecular Formula: C₉H₁₂O₆

Molecular Weight: 216.19

Accurate Mass: 216.06339

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

Melting Point: Mp 157.5-158°

>>Variant: (1 α ,2 α ,3 β)-form

Synonym(s): *trans*-form

CAS Registry Number: 705-35-1

Molecular Formula: C₆H₆O₆

Molecular Weight: 174.11

Accurate Mass: 174.01644

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

Physical Description: Needles (H₂O)

Melting Point: Mp 220°

Solubility: Sol. H₂O

pKa Value: pK_{a1} 2.8; pK_{a2} 4.1; pK_{a3} 6.4

>>Derivative: Tri-Me ester

CAS Registry Number: 717-69-1

Melting Point: Mp 58°

Boiling Point: Bp₁₈₀ 224°

>>Derivative: Di-Me ester, amide

Molecular Formula: C₈H₁₁NO₅

Molecular Weight: 201.179

Accurate Mass: 201.063724

Percentage Composition: C 47.76%; H 5.51%; N 6.96%; O 39.76%

Melting Point: Mp 185°

References:

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Grundmann, C., *Annalen*, 1943, **555**, 77, (*synth*)

Church, J.F. *et al.*, *Chem. Ind. (London)*, 1962, 1574, (*cryst struct*)

Ettlinger, M.G. *et al.*, *Chem. Ind. (London)*, 1962, 1574, (*synth*)

Jones, P.G. *et al.*, *Acta Cryst. C*, 1987, **43**, 1179, (*cryst struct, nitrile*)