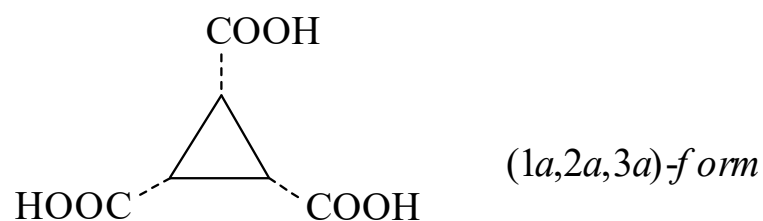




>>Entry Name: 1,2,3-Cyclopropanetricarboxylic acid, 9CI

Synonym(s): Aceconitic acid



**Molecular Formula:** C<sub>6</sub>H<sub>6</sub>O<sub>6</sub>

**Molecular Weight:** 174.11

**Accurate Mass:** 174.01644

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

>>Variant: (1 $\alpha$ ,2 $\alpha$ ,3 $\alpha$ )-form

Synonym(s): *cis*-form

**Molecular Formula:** C<sub>6</sub>H<sub>6</sub>O<sub>6</sub>

**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<sub>a2</sub> 4.5; pK<sub>a3</sub> 10

>>Derivative: Tri-Me ester

**Molecular Formula:** C<sub>9</sub>H<sub>12</sub>O<sub>6</sub>

**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 $\alpha$ ,2 $\alpha$ ,3 $\beta$ )-form

Synonym(s): *trans*-form

**CAS Registry Number:** 705-35-1

**Molecular Formula:** C<sub>6</sub>H<sub>6</sub>O<sub>6</sub>

**Molecular Weight:** 174.11

**Accurate Mass:** 174.01644

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

**Physical Description:** Needles (H<sub>2</sub>O)

**Melting Point:** Mp 220°

**Solubility:** Sol. H<sub>2</sub>O

**pKa Value:** pK<sub>a1</sub> 2.8; pK<sub>a2</sub> 4.1; pK<sub>a3</sub> 6.4

>>Derivative: Tri-Me ester

**CAS Registry Number:** 717-69-1

**Melting Point:** Mp 58°

**Boiling Point:** Bp<sub>180</sub> 224°

>>Derivative: Di-Me ester, amide

**Molecular Formula:** C<sub>8</sub>H<sub>11</sub>NO<sub>5</sub>

**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:

Buchner, E. *et al.*, *Ber.*, 1890, **23**, 2584

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*)