



**Melting Point:** Mp 156-157°

**Optical Rotation:**  $[\alpha]_D +60.9$  (H<sub>2</sub>O)

>>**Variant:** (1*RS*,2*RS*)-form

**Synonym(s):** (±)-*erythro*-form. (±)-Alloisocitric acid

**CAS Registry Number:** 344-79-6

**Molecular Formula:** C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>

**Molecular Weight:** 192.125

**Accurate Mass:** 192.027005

**Percentage Composition:** C 37.51%; H 4.20%; O 58.29%

>>**Derivative:** 1,4-Lactone

**CAS Registry Number:** 3118-83-0

**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 153°

>>**Variant:** (1*RS*,2*SR*)-form

**Synonym(s):** (±)-*threo*-form. (±)-Isocitric acid

**CAS Registry Number:** 18979-21-0

**Molecular Formula:** C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>

**Molecular Weight:** 192.125

**Accurate Mass:** 192.027005

**Percentage Composition:** C 37.51%; H 4.20%; O 58.29%

>>**Derivative:** 1,4-Lactone

**CAS Registry Number:** 4702-32-3

**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 161°

**Aldrich:** I-1600-5

**Fluka:** 58780

**Sigma:** I1377

#### References:

*Aldrich Library of <sup>13</sup>C and <sup>1</sup>H FT NMR Spectra*, 1992, **1**, 1145A, (*nmr*)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 704C, (*ir, lactone*)

Kaneko, T. *et al.*, *Chem. Ind. (London)*, 1960, 1187; 1188, (*struct*)

Vickery, H.B., *J. Biol. Chem.*, 1962, **237**, 1739, (*nomencl*)

Patterson, A.L. *et al.*, *J.A.C.S.*, 1962, **84**, 309, (*cryst struct*)

Clark, R.B., *Crop Sci.*, 1969, **9**, 341, (*isol*)

Lehninger, A.L. *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, 1978, **75**, 1690, (*metab*)