



Melting Point: Mp 156-157°

Optical Rotation: $[\alpha]_D +60.9$ (H₂O)

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

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

CAS Registry Number: 344-79-6

Molecular Formula: C₆H₈O₇

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: C₆H₆O₆

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: C₆H₈O₇

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: C₆H₆O₆

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 ¹³C and ¹H 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*)