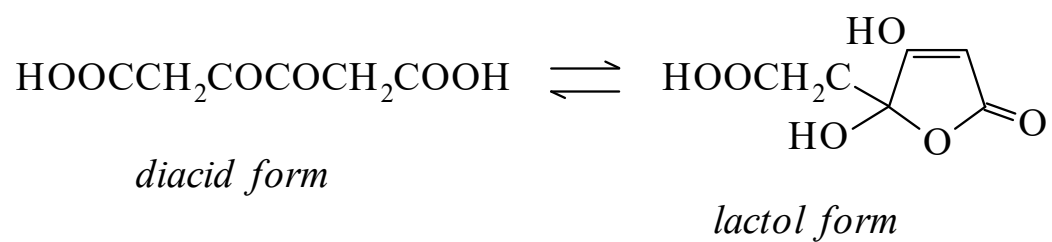




>>Entry Name: 3,4-Dioxohexanedioic acid, 9CI

Synonym(s): 3,4-Dihydroxy-2,4-hexadienedioic acid. 3,4-Dioxoadipic acid. Ketipic acid. 2,3-Dioxobutanedicarboxylic acid. Oxalodiacetic acid



CAS Registry Number: 533-76-6

Molecular Formula: C₆H₆O₆

Molecular Weight: 174.11

Accurate Mass: 174.01644

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

General Statement: Exists in soln. as lactol form

Physical Description: Amorph. powder

Solubility: Sol. conc. HCl, AcOH, spar. sol. Et₂O, insol. H₂O, EtOH, C₆H₆

Other Data: Dec. at 150°

>>Derivative: Di-Et ester

CAS Registry Number: 3249-69-2

Molecular Formula: C₁₀H₁₄O₆

Molecular Weight: 230.217

Accurate Mass: 230.07904

Percentage Composition: C 52.17%; H 6.13%; O 41.70%

Physical Description: Prisms (EtOH)

Melting Point: Mp 82-83° (76-77°)

Rare Chemicals Library: S1714-1

>>Derivative: Di-*tert*-butyl ester

Molecular Formula: C₁₄H₂₂O₆

Molecular Weight: 286.324

Accurate Mass: 286.14164

Percentage Composition: C 58.73%; H 7.74%; O 33.53%

Physical Description: Needles

Melting Point: Mp 121 dec.°

References:

Fanzen, H. *et al.*, *Ber.*, 1925, **58**, 224, (*synth*)

Stachel, H.-D. *et al.*, *Annalen*, 1965, **689**, 118, (*ir, pmr, tautom*)