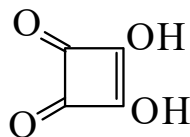




>>Entry Name: 3,4-Dihydroxy-3-cyclobutene-1,2-dione, 9CI

Synonym(s): Squaric acid. 1,2-Dihydroxycyclobutenedione. Quadratic acid. Diketocyclobutenediol



CAS Registry Number: 2892-51-5

Molecular Formula: C₄H₂O₄

Molecular Weight: 114.057

Accurate Mass: 113.99531

Percentage Composition: C 42.12%; H 1.77%; O 56.11%

Use/Importance: Used for photometric detn. of Cu, Fe(III), U(VI) ($\lambda_{\max}$ 400 nm, ϵ 1450)

Physical Description: Cryst. (H₂O)

Melting Point: Mp 293 dec. approx.°

Solubility: Sol. H₂O

pKa Value: pK_{a1} 0.55; pK_{a2} 3.48 (25°)

Other Data: $\lambda_{\max}$ 269.5 nm (ϵ 37000)

Aldrich: 23104-5

Fluka: 37670

Sigma: S2756

>>Derivative: Mono-Me ester

Synonym(s): 1-Hydroxy-2-methoxycyclobutenedione

CAS Registry Number: 5231-86-7

Molecular Formula: C₅H₄O₄

Molecular Weight: 128.084

Accurate Mass: 128.01096

Percentage Composition: C 46.89%; H 3.15%; O 49.97%

Physical Description: Solid

Melting Point: Mp 132-134°

>>Derivative: Di-Me ester

Synonym(s): 1,2-Dimethoxycyclobutenedione

CAS Registry Number: 5222-73-1

Molecular Formula: C₆H₆O₄

Molecular Weight: 142.111

Accurate Mass: 142.02661

Percentage Composition: C 50.71%; H 4.26%; O 45.03%

Use/Importance: Reagent for preparation of glycoconjugates

Physical Description: Fluffy-white cryst. (Et₂O)

Melting Point: Mp 56.7-56.8°

Aldrich: 37740-6

>>Derivative: Di-Et ester

Synonym(s): 1,2-Diethoxycyclobutenedione

CAS Registry Number: 5231-87-8

Molecular Formula: C₈H₁₀O₄

Molecular Weight: 170.165

Accurate Mass: 170.05791

Percentage Composition: C 56.47%; H 5.92%; O 37.61%

Use/Importance: Reagent for preparing glycoconjugates

Biological Use/Importance: Has fungicidal props. Contact sensitiser. Used to treat alopecia areata

Boiling Point: Bp_{0.4} 88-91°

Aldrich: 31077-8

Fluka: 31630