



Physical Description: Needles (Et₂O/petrol)

Melting Point: Mp 93.5 dec.°

Solubility: Sol. H₂O, Et₂O; insol. C₆H₆, CS₂, petrol

pKa Value: pK_{a1} 2.2; pK_{a2} 5.6 (25°, 0.1M NaClO₄) pK_{a1} 2.8; pK_{a2} 6.1 (25°)

Other Data: Steam-volatile with formation of anhydride. Dist. → anhydride. Isom. by sunlight + trace of Br₂ → (Z)-form. Citraconic acid and its esters undergo radical copolym. with vinyl monomers, e.g. styrene

Hazard & Toxicity: LD₅₀ (rat, orl) 1320 mg/kg

Aldrich: C8260-4

Fluka: 27420

Sigma: C9404

>>Derivative: Di-Me ester

CAS Registry Number: 617-54-9

Molecular Formula: C₇H₁₀O₄

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Boiling Point: Bp 210-211°. Bp₁₀ 92.8°

Solubility: V. sol. Me₂CO, Et₂O, EtOH

Density: d²⁰ 1.1153

Refractive Index: n_D²⁰ 1.4473

>>Derivative: Di-Et ester

CAS Registry Number: 691-83-8

Boiling Point: Bp 230.3°. Bp₂₀ 120°

Solubility: Sol. EtOH, Et₂O

Density: d²⁰ 1.0431

Refractive Index: n_D²⁰ 1.4468

>>Derivative: Dichloride

Molecular Formula: C₅H₄Cl₂O₂

Molecular Weight: 166.991

Accurate Mass: 165.958834

Percentage Composition: C 35.96%; H 2.41%; Cl 42.46%; O 19.16%

Boiling Point: Bp₁₈ 95°

>>Derivative: Anhydride

Synonym(s): 3-Methyl-2,5-furandione, 9Cl. Citraconic anhydride

CAS Registry Number: 616-02-4

Molecular Formula: C₅H₄O₃

Molecular Weight: 112.085

Accurate Mass: 112.016045

Percentage Composition: C 53.58%; H 3.60%; O 42.82%

Melting Point: Mp 7°

Boiling Point: Bp 213°

Solubility: V. sol. EtOH, Me₂CO, Et₂O

Density: d¹⁶ 1.2469

Refractive Index: n_D²¹ 1.4710

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 2600 mg/kg; LD₅₀ (rbt, skn) 218 mg/kg

Aldrich: 12531-8

Fluka: 27440

Sigma: C2395

>>Derivative: Diamide

CAS Registry Number: 41138-17-4

Melting Point: Mp 185-187 dec.°

Other Data: Forms imide at Mp

>>Derivative: 4-Anilide