



>>Entry Name: Dichloroacetic acid, 9Cl

Synonym(s): Dichloroethanoic acid

CAS Registry Number: 79-43-6

Related CAS Registry Numbers(s): 2156-56-1 13425-80-4

Cl₂CHCOOH

Molecular Formula: C₂H₂Cl₂O₂

Molecular Weight: 128.942

Accurate Mass: 127.943184

Percentage Composition: C 18.63%; H 1.56%; Cl 54.99%; O 24.82%

Biological Use/Importance: Has fungicidal props.

Physical Description: Corrosive liq.

Melting Point: Mp 5-6° (11°)

Boiling Point: Bp 194°. Bp₂₀ 102°

Solubility: Misc. H₂O, EtOH

Density: d₄²⁰ 1.563

Refractive Index: n_D²² 1.4659

Hazard & Toxicity: Fl. p. >66°. Corrosive and irritating to all tissues. LD₅₀ (rbt, skn) 510 mg/kg

Aldrich: D5470-2

Fluka: 35810

Sigma: D5932

Supelco: R47-2665

>>Derivative: Na salt

Synonym(s): Sodium dichloroacetate, USAN. Ceresine. CPC 211

CAS Registry Number: 2156-56-1

Biological Use/Importance: Pyruvate dehydrogenase activator. Used in the treatment of neurologic injury

>>Derivative: Me ester

CAS Registry Number: 116-54-1

Molecular Formula: C₃H₄Cl₂O₂

Molecular Weight: 142.969

Accurate Mass: 141.958834

Percentage Composition: C 25.20%; H 2.82%; Cl 49.60%; O 22.38%

Physical Description: Liq.

Boiling Point: Bp 143-144°

Hazard & Toxicity: Skin, eye, and mucous membrane irritant

Aldrich: 10840-5

Fluka: 35840

Supelco: R30-2705

>>Derivative: Et ester

CAS Registry Number: 535-15-9

Molecular Formula: C₄H₆Cl₂O₂

Molecular Weight: 156.996

Accurate Mass: 155.974484

Percentage Composition: C 30.60%; H 3.85%; Cl 45.16%; O 20.38%

Boiling Point: Bp 155-158°

Density: d₄²⁰ 1.31. d₄²⁰ 1.28

Refractive Index: n_D²⁰ 1.4386

Fluka: 35820

Rare Chemicals Library: S70601-9