



>>Entry Name: Tribromoacetic acid, 9CI, 8CI

CAS Registry Number: 75-96-7

Br₃CCOOH

Molecular Formula: C₂HBr₃O₂

Molecular Weight: 296.741

Accurate Mass: 293.812663

Percentage Composition: C 8.10%; H 0.34%; Br 80.78%; O 10.78%

Physical Description: Monoclinic prisms

Melting Point: Mp 131°

Boiling Point: Bp 245° dec.

Solubility: Sol. H₂O, EtOH, Et₂O

pKa Value: pK_a 0.66 (25°, H₂O)

Hazard & Toxicity: Irritant

Aldrich: T4820-8

Fluka: 90720

Supelco: R47-3420

>>Derivative: Me ester

CAS Registry Number: 3222-05-7

Molecular Formula: C₃H₃Br₃O₂

Molecular Weight: 310.768

Accurate Mass: 307.828313

Percentage Composition: C 11.59%; H 0.97%; Br 77.14%; O 10.30%

Boiling Point: Bp₁₅ 103°

Density: d 2.33

Refractive Index: n_D²⁰ 1.5580

>>Derivative: Et ester

CAS Registry Number: 599-99-5

Molecular Formula: C₄H₅Br₃O₂

Molecular Weight: 324.794

Accurate Mass: 321.843963

Percentage Composition: C 14.79%; H 1.55%; Br 73.80%; O 9.85%

Physical Description: Liq.

Boiling Point: Bp 178-180°. Bp₇₃ 148°

>>Derivative: Chloride

CAS Registry Number: 34718-47-3

Molecular Formula: C₂Br₃ClO

Molecular Weight: 315.186

Accurate Mass: 311.778775

Percentage Composition: C 7.62%; Br 76.05%; Cl 11.25%; O 5.08%

Physical Description: Liq.

Boiling Point: Bp₁₂ 80-82°

Aldrich: 43165-6

>>Derivative: Bromide

CAS Registry Number: 10588-31-5

Molecular Formula: C₂Br₄O

Molecular Weight: 359.637

Accurate Mass: 355.748259

Percentage Composition: C 6.68%; Br 88.87%; O 4.45%

Physical Description: Liq.

Boiling Point: Bp 210-215°. Bp₁₂ 88-90°