



>>Entry Name: Nitroacetic acid, 9Cl, 8Cl

CAS Registry Number: 625-75-2

O₂NCH₂COOH

Molecular Formula: C₂H₃NO₄

Molecular Weight: 105.05

Accurate Mass: 105.006209

Percentage Composition: C 22.87%; H 2.88%; N 13.33%; O 60.92%

Physical Description: Needles (CHCl₃)

Melting Point: Mp 87-89 dec.°

Solubility: V. sol. EtOH, Et₂O, insol. petrol

pKa Value: pK_a 1.68

Other Data: Heated with H₂O → Nitromethane [CVV41-Y](#)

>>Derivative: Me ester

CAS Registry Number: 2483-57-0

Molecular Formula: C₃H₅NO₄

Molecular Weight: 119.077

Accurate Mass: 119.021859

Percentage Composition: C 30.26%; H 4.23%; N 11.76%; O 53.74%

Physical Description: Liq.

Boiling Point: Bp₂₈ 107°. Bp_{3,5} 69.5-71.5°

Solubility: Spar. sol. H₂O

Density: d₄⁰ 1.32

Aldrich: 36646-3

Fluka: 73325

>>Derivative: Et ester

CAS Registry Number: 626-35-7

Molecular Formula: C₄H₇NO₄

Molecular Weight: 133.104

Accurate Mass: 133.037509

Percentage Composition: C 36.10%; H 5.30%; N 10.52%; O 48.08%

Physical Description: Liq.

Boiling Point: Bp_{1,5} 70°

Aldrich: 19233-3

Fluka: 73315

>>Derivative: Isopropyl ester

CAS Registry Number: 31333-37-6

Molecular Formula: C₅H₉NO₄

Molecular Weight: 147.13

Accurate Mass: 147.053159

Percentage Composition: C 40.82%; H 6.17%; N 9.52%; O 43.50%

Physical Description: Liq.

Boiling Point: Bp_{0,9} 52°

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 18598-93-1

Molecular Formula: C₆H₁₁NO₄

Molecular Weight: 161.157

Accurate Mass: 161.068809

Percentage Composition: C 44.72%; H 6.88%; N 8.69%; O 39.71%

Physical Description: Liq.

Boiling Point: Bp₄ 74°

>>Derivative: Amide

Synonym(s): Nitroacetamide