



>>Entry Name: (4-Nitrophenoxy)acetic acid, 9CI

Synonym(s): (4-Nitrophenoxy)ethanoic acid. Glycollic acid 4-nitrophenyl ether

CAS Registry Number: 1798-11-4

Molecular Formula: C₈H₇NO₅

Molecular Weight: 197.147

Accurate Mass: 197.032424

Percentage Composition: C 48.74%; H 3.58%; N 7.10%; O 40.58%

Use/Importance: Potential herbicide, fungicide

Physical Description: Leaflets (MeOH or EtOH)

Melting Point: Mp 187.2-187.5°

pKa Value: pK_{a1} 2.81 (25°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 936 mg/kg

Rare Chemicals Library: S38506-9

>>Derivative: Me ester

CAS Registry Number: 19786-48-2

Molecular Formula: C₉H₉NO₅

Molecular Weight: 211.174

Accurate Mass: 211.048074

Percentage Composition: C 51.19%; H 4.30%; N 6.63%; O 37.88%

Melting Point: Mp 100-101°

>>Derivative: Et ester

CAS Registry Number: 19076-89-2

Molecular Formula: C₁₀H₁₁NO₅

Molecular Weight: 225.201

Accurate Mass: 225.063724

Percentage Composition: C 53.33%; H 4.92%; N 6.22%; O 35.52%

Physical Description: Pale-yellow leaflets (EtOH)

Melting Point: Mp 75-76°

Boiling Point: Bp₁₅ 203-206°

Rare Chemicals Library: S65299-7

>>Derivative: Chloride

CAS Registry Number: 20142-88-5

Molecular Formula: C₈H₆ClNO₄

Molecular Weight: 215.592

Accurate Mass: 214.998536

Percentage Composition: C 44.57%; H 2.81%; Cl 16.44%; N 6.50%; O 29.68%

Physical Description: Plates or prisms (C₆H₆)

Melting Point: Mp 86-87°

>>Derivative: Amide

CAS Registry Number: 63218-14-4

Molecular Formula: C₈H₈N₂O₄

Molecular Weight: 196.162

Accurate Mass: 196.048408

Percentage Composition: C 48.98%; H 4.11%; N 14.28%; O 32.62%

Physical Description: Prisms or needles

Melting Point: Mp 156-158°

References: