



>>Entry Name: (3-Nitrophenoxy)acetic acid, 9Cl

Synonym(s): (3-Nitrophenoxy)ethanoic acid. Glycollic acid 3-nitrophenyl ether

CAS Registry Number: 1878-88-2

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: Has fungicidal props.

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 156.4-156.7°

pKa Value: pK_{a1} 2.91 (25°)

>>Derivative: Me ester

CAS Registry Number: 7506-93-6

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%

Physical Description: Needles

Melting Point: Mp 66.5°

>>Derivative: Et ester

CAS Registry Number: 5544-77-4

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: Yellow liq.

Boiling Point: Bp₃₀ 208-212°

>>Derivative: Chloride

CAS Registry Number: 40257-02-1

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: Prisms (C₆H₆)

Melting Point: Mp 49-51°

>>Derivative: Amide

CAS Registry Number: 90370-49-3

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: Yellow prisms

Melting Point: Mp 178.5°

References:

Jacobs, W.A. *et al.*, *J.A.C.S.*, 1917, **39**, 2188-2224, (*synth*)

Zawadowska, I., *Acta Pol. Pharm.*, 1962, **19**, 263-267, (*synth, pharmacol*)

Deshmukh, J.G. *et al.*, *Synth. Commun.*, 1986, **16**, 479-483, (*synth*)

Takeda, Y. *et al.*, *Chem. Pharm. Bull.*, 1998, **46**, 434-444, (*esters, synth, pmr*)

Asagarasu, A. *et al.*, *Chem. Pharm. Bull.*, 1998, **46**, 697-703, (*synth, pmr*)