



>>Entry Name: Phenoxyacetic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Glycollic acid phenyl ether. FEMA 2872

CAS Registry Number: 122-59-8

PhOCH₂COOH

Molecular Formula: C₈H₈O₃

Molecular Weight: 152.149

Accurate Mass: 152.047345

Percentage Composition: C 63.15%; H 5.30%; O 31.55%

Biological Source: Prod. by *Aspergillus niger*. Present in cocoa beans

Use/Importance: Flavouring ingredient

Physical Description: Needles (H₂O) with sour, sweet odour and honey-like taste

Melting Point: Mp 98-99°

Boiling Point: Bp 285° dec.

pKa Value: pK_{a1} 3.16 (25°) pK_a 5.12

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 1500 mg/kg

Aldrich: W28720-2

Fluka: 77740

Sigma: P1001

>>Derivative: Me ester

CAS Registry Number: 2065-23-8

Molecular Formula: C₉H₁₀O₃

Molecular Weight: 166.176

Accurate Mass: 166.062995

Percentage Composition: C 65.05%; H 6.07%; O 28.88%

Boiling Point: Bp 245°

Aldrich: 27563-8

Sigma: P9782

>>Derivative: Et ester

CAS Registry Number: 2555-49-9

Molecular Formula: C₁₀H₁₂O₃

Molecular Weight: 180.203

Accurate Mass: 180.078645

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

Physical Description: Oil

Boiling Point: Bp 250-251°. Bp_{0.05} 84°

Aldrich: 46293-4

Rare Chemicals Library: S67276-9

Other: Oakwood 1014

>>Derivative: 2-Propenyl ester

Synonym(s): Allyl phenoxyacetate. FEMA 2038

CAS Registry Number: 7493-74-5

Molecular Formula: C₁₁H₁₂O₃

Molecular Weight: 192.214

Accurate Mass: 192.078645

Percentage Composition: C 68.74%; H 6.29%; O 24.97%

Use/Importance: Flavouring ingredient

Physical Description: Liq. with honey and pineapple-like aroma

Boiling Point: Bp₁ 100-102°

Refractive Index: n_D^{25.5} 1.5131

Hazard & Toxicity: LD₅₀ (rat, orl) 475 mg/kg. LD₅₀ (rbt, skn) 820 mg/kg

Aldrich: W20380-7