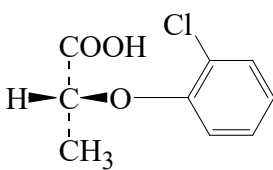




>>Entry Name: 2-(2-Chlorophenoxy)propanoic acid, 9Cl



(*R*)-form

CAS Registry Number: 25140-86-7

Related CAS Registry Numbers(s): 52094-99-2 74411-15-7 109423-86-1 109583-03-1 122674-93-5 133707-33-2

Molecular Formula: C₉H₉ClO₃

Molecular Weight: 200.621

Accurate Mass: 200.024022

Percentage Composition: C 53.88%; H 4.52%; Cl 17.67%; O 23.92%

Aldrich: 22589-4

>>Variant: (*R*)-form

CAS Registry Number: 31460-41-0

Molecular Formula: C₉H₉ClO₃

Molecular Weight: 200.621

Accurate Mass: 200.024022

Percentage Composition: C 53.88%; H 4.52%; Cl 17.67%; O 23.92%

Physical Description: Needles (HCOOH aq.)

Melting Point: Mp 95-95.5°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +30.2$ (c, 2.04 in Me₂CO)

>>Variant: (*S*)-form

CAS Registry Number: 31460-42-1

Molecular Formula: C₉H₉ClO₃

Molecular Weight: 200.621

Accurate Mass: 200.024022

Percentage Composition: C 53.88%; H 4.52%; Cl 17.67%; O 23.92%

Physical Description: Needles (HCOOH aq.)

Melting Point: Mp 95-95.5°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -30.1$ (c, 2.04 in Me₂CO). $[\alpha]_{\text{D}}^{25} -1.23$ (c, 2.03 in EtOH)

>>Variant: (±)-form

CAS Registry Number: 76466-16-5

Molecular Formula: C₉H₉ClO₃

Molecular Weight: 200.621

Accurate Mass: 200.024022

Percentage Composition: C 53.88%; H 4.52%; Cl 17.67%; O 23.92%

Melting Point: Mp 114-115°

>>Derivative: Me ester

CAS Registry Number: 122623-80-7

Molecular Formula: C₁₀H₁₁ClO₃

Molecular Weight: 214.648

Accurate Mass: 214.039672

Percentage Composition: C 55.96%; H 5.17%; Cl 16.52%; O 22.36%

Boiling Point: Bp_{0.7} 97-98°

References:

Fredga, A. *et al.*, *Ark. Kemi*, 1961, **17**, 265, (*synth, resoln*)

Gabard, J. *et al.*, *Nouv. J. Chim.*, 1986, **10**, 685, (*R-form synth*)

Pettersson, C. *et al.*, *J. Chromatogr.*, 1987, **398**, 247, (*chiral hplc*)

Denoncour, R. *et al.*, *J. Chromatogr.*, 1987, **410**, 355, (*Me ester chiral hplc*)

Chenevert, R. *et al.*, *Can. J. Chem.*, 1988, **66**, 1219, (*resoln*)