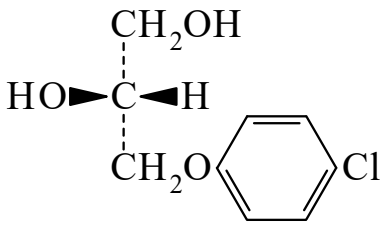
>>**Entry Name: 3-(4-Chlorophenoxy)-1,2-propanediol,** 9Cl
Synonym(s): Chlorphenesin, BAN, INN**.** Adermykon. Demykon. Fungimixin. Gecophen. Kolpicortin-sine. Mycil. Nycil. Soorphenesin



(*R*)-*form*

CAS Registry Number: 104-29-0

Molecular Formula: $C_9H_{11}ClO_3$
Molecular Weight: 202.637
Accurate Mass: 202.039672
Percentage Composition: C 53.35%; H 5.47%; Cl 17.50%; O 23.69%
Use/Importance: Skeletal muscle relaxant and fungicide
Calculated Log P Data: Log P 1.22 (calc)

Rare Chemicals Library: S42764-0

>>**Variant:** (*R*)-form

Molecular Formula: $C_9H_{11}ClO_3$
Molecular Weight: 202.637
Accurate Mass: 202.039672
Percentage Composition: C 53.35%; H 5.47%; Cl 17.50%; O 23.69%
Optical Rotation: $[\alpha]_D$ –11.8 (c, 1 in EtOH) (95% ee)

>>**Variant:** (*S*)-form

Molecular Formula: $C_9H_{11}ClO_3$
Molecular Weight: 202.637
Accurate Mass: 202.039672
Percentage Composition: C 53.35%; H 5.47%; Cl 17.50%; O 23.69%
Optical Rotation: $[\alpha]_D$ +12.3 (c, 1 in EtOH) (97% ee)

>>**Variant:** (±)-form

Molecular Formula: $C_9H_{11}ClO_3$
Molecular Weight: 202.637
Accurate Mass: 202.039672
Percentage Composition: C 53.35%; H 5.47%; Cl 17.50%; O 23.69%
Melting Point: Mp 77-79°

>>**Derivative:** 1-Carbamate
Synonym(s): Chlorphenesin carbamate, JAN, USAN**.** Maolate. Rinlaxer. U 19646

CAS Registry Number: 886-74-8
Molecular Formula: $C_{10}H_{12}ClNO_4$
Molecular Weight: 245.662
Accurate Mass: 245.045486
Percentage Composition: C 48.89%; H 4.92%; Cl 14.43%; N 5.70%; O 26.05%
Use/Importance: Skeletal muscle relaxant
Physical Description: Cryst. (C_6H_6/toluene)
Melting Point: Mp 89-91°
Solubility: Insol. H_2O, C_6H_6, cyclohexane, sol. dioxan
Calculated Log P Data: Log P 1.26 (calc)
Hazard & Toxicity: CNS depressant which causes drowsiness and other adverse effects. LD_{50} (rat, orl) 632 mg/kg. Exp. reprod. effects

References: