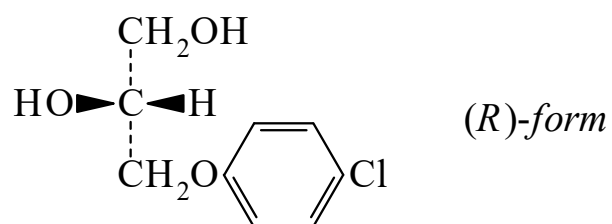




>>Entry Name: 3-(4-Chlorophenoxy)-1,2-propanediol, 9Cl

Synonym(s): Chlorphenesin, BAN, INN. Adermykon. Demykon. Fungimixin. Gecophen. Kolpicortin-sine. Mycil. Nycil. Soorphenesin



CAS Registry Number: 104-29-0

Molecular Formula: C₉H₁₁ClO₃

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: C₉H₁₁ClO₃

Molecular Weight: 202.637

Accurate Mass: 202.039672

Percentage Composition: C 53.35%; H 5.47%; Cl 17.50%; O 23.69%

Optical Rotation: [α]_D −11.8 (c, 1 in EtOH) (95% ee)

>>Variant: (S)-form

Molecular Formula: C₉H₁₁ClO₃

Molecular Weight: 202.637

Accurate Mass: 202.039672

Percentage Composition: C 53.35%; H 5.47%; Cl 17.50%; O 23.69%

Optical Rotation: [α]_D +12.3 (c, 1 in EtOH) (97% ee)

>>Variant: (±)-form

Molecular Formula: C₉H₁₁ClO₃

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: C₁₀H₁₂ClNO₄

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. (C₆H₆/toluene)

Melting Point: Mp 89-91°

Solubility: Insol. H₂O, C₆H₆, cyclohexane, sol. dioxan

Calculated Log P Data: Log P 1.26 (calc)

Hazard & Toxicity: CNS depressant which causes drowsiness and other adverse effects. LD₅₀ (rat, orl) 632 mg/kg. Exp. reprod. effects

References: