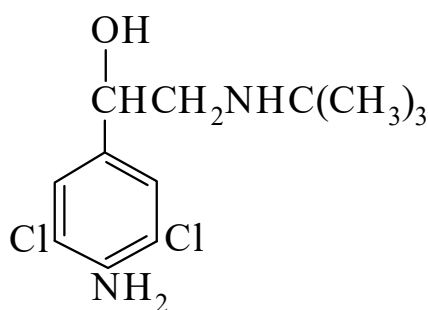




>>Entry Name: Clenbuterol, BAN, INN

ENTRY UNDER REVIEW

Synonym(s): 4-Amino-3,5-dichloro- α -[[[(1,1-dimethylethyl)amino]methyl]benzenemethanol, 9Cl. 1-(4-Amino-3,5-dichlorophenyl)-2-*tert*-butylaminoethanol. Spiropent. Ventipulmin. NAB 365. Many other names



CAS Registry Number: 37148-27-9

Related CAS Registry Numbers(s): 21898-19-1

Molecular Formula: C₁₂H₁₈Cl₂N₂O

Molecular Weight: 277.192

Accurate Mass: 276.079617

Percentage Composition: C 52.00%; H 6.54%; Cl 25.58%; N 10.11%; O 5.77%

Use/Importance: Potential food contaminant arising from its illicit use to improve carcass quality and productivity in cattle. Approved tocolytic agent for cows in several European countries

Biological Use/Importance: β -Adrenoceptor agonist. Bronchodilator, uterine relaxant

Calculated Log P Data: Log P 2.38 (calc)

Hazard & Toxicity: LD₅₀ (rat,orl) 159 mg/kg. Exp. reprod. and teratogenic effects

>>Variant: (+)-form

CAS Registry Number: 50499-60-0

Molecular Formula: C₁₂H₁₈Cl₂N₂O

Molecular Weight: 277.192

Accurate Mass: 276.079617

Percentage Composition: C 52.00%; H 6.54%; Cl 25.58%; N 10.11%; O 5.77%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 127-128.5°

Optical Rotation: [α]₃₆₄²⁰ +244 (c, 2.28 in CHCl₃)

Other Data: Abs. configs. not detd. (1994)

>>Derivative: Hydrochloride

CAS Registry Number: 50310-83-3

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 197.5-198°

Optical Rotation: [α]₃₆₄²⁰ +126 (c, 2.15 in H₂O)

>>Variant: (–)-form

CAS Registry Number: 50306-03-1

Molecular Formula: C₁₂H₁₈Cl₂N₂O

Molecular Weight: 277.192

Accurate Mass: 276.079617

Percentage Composition: C 52.00%; H 6.54%; Cl 25.58%; N 10.11%; O 5.77%

Physical Description: Cryst. (H₂O)

Optical Rotation: [α]₃₆₄²⁰ –243 (c, 2.65 in CHCl₃)

Other Data: Active isomer

>>Derivative: Hydrochloride

CAS Registry Number: 50310-85-5

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 187-188 dec.°

Optical Rotation: [α]₃₆₄²⁰ –126 (c, 2.72 in H₂O)