



Formula: C₉H₁₃NO₂

MW: 167.21

Salt: HCl

CAS: 61-76-7

MDL NUMBER: MFCD00063028

IUPAC: 1-(3-hydroxyphenyl)-2-(methylamino)ethan-1-ol

Smiles: c1cc(cc(c1)O)C(CNC)O

L(-)-Phenylephrine hydrochloride 99%

THERAPEUTIC CATEGORY: Phenylephrine or neosynephrine is an α -adrenergic receptor agonist used primarily as a decongestant, as an agent to dilate the pupil, and rarely to increase blood pressure.

ACCEPTORS: 2

DONORS: 3

ROTATION BONDS: 5

N+O: 3

Chiral Centers: 1

LogP: 0.54

LogS: -2.63

LIPINSKI: 4

Synonyms:

(-)-alpha-hydroxy-beta-(methylamino)ethyl-alpha-(3-hydroxybenzene)hydrochlor;1-m-hydroxy-alpha-(methylaminomethyl)benzylalcoholhydrochloride;3-hydroxy-alpha-((methylamino)methyl)-hydrochloride,(-)-benzenemethanol;almefrin;benzenemethanol,3-hydroxy-alpha-[(methylamino)methyl]-hydrochloride,(thet;consdrin;consdrinhydrochloride;d(-)-phenylephrinehydrochloride

CAS:61-76-7

MF:C9H14ClNO2

MW:203.67

EINECS:200-517-3

Product Categories: Phenylephrine hydrochloride

Chemical Properties: mp 143-145 C(lit.) alpha -47 (c=2, H2O) refractive index -45.5 (C=1, H2O) storage temp. Desiccate at RT Water Solubility >=10 g/100 mL at 21 C Merck 7286

CAS DataBase Reference: 61-76-7(

CAS DataBase Reference:) EPA Substance Registry System Benzenemethanol, 3-hydroxy-.alpha-[(methylamino) methyl]-, hydrochloride, (.alpha.R)-(61-76-7) Xn Risk Statements 22-36/37/38 Safety Statements 26-36-37/39 RIDADR 3249 WGK Germany 3 RTECS DO7525000 HazardClass 6.1(b) PackingGroup III (R)-(-)-1-(3-Hydroxyphenyl)-2-methylaminoethanol hydrochloride Phenylephrine hydrochloride

Usage And Synthesis:

Chemical Properties: white to almost white crystalline powder General Description Odorless white microcrystalline powder. Bitter taste. pH (1% aqueous solution) about 5. Air & Water Reactions May be sensitive to prolonged exposure to air and light. Water soluble. Reactivity Profile Phenylephrine hydrochloride is incompatible with acids, acid chlorides, acid anhydrides and oxidizing agents. Phenylephrine hydrochloride is also incompatible with butacaine, alkalis and ferric salts. Fire Hazard Flash point data for Phenylephrine hydrochloride are not available; however, Phenylephrine hydrochloride is probably combustible. Biological Activity a 1 -adrenoceptor agonist; pK i values are 5.86, 4.87 and 4.70 for a 1D , a 1B and a 1A receptors respectively. Phenylephrine hydrochloride

