



Formula: C₂₇H₃₉ClN₂O₄

MW: 491.07

CAS: 23313-68-0

TNP NUMBER: TNP00358

MDL NUMBER: MFCD00055208

IUPAC: 2-(3,4-dimethoxyphenyl)-5-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]-2-(methyl)pentanenitrile, chloride

Smiles: C(C(C(C)C)(C#N)c1cc(OC)c(cc1)OC)CCN(CCc1cc(OC)c(cc1)OC)C.Cl

THERAPEUTIC CATEGORY: Antihypertensive, antianginal, antiarrhythmic

REFERENCE: Merck 13, 10012

ACCEPTORS: 4

DONORS: 0

ROTATION BONDS: 13

N+O: 6

Chiral Centers: 1

LogP: 6.36

LogS: -6.24

LIPINSKI: 3

Synonyms:

CALAN;IPROVERATRIL;ISOPTIN;(±)-5-[N-(3,4-DIMETHOXYPHENYLETHYL)-METHYLAMINO]-2-(3,4-DIMETHOXYPHENYL)-2-ISOPROPYLVALERONITRILE HYDROCHLORIDE;5-[N-(3,4-DIMETHOXYPHENYLETHYL)METHYLAMINO]-2-(3,4-DIMETHOXYPHENYL)-2-ISOPROPYLVALERONITRILE HYDROCHLORIDE;alpha-(3-((2-(3,4-dimethoxyphenyl)ethyl)methylamino)propyl)-3,4-dimethoxy-alpha-(1-methylethyl)-benzeneacetonitrile hydrochloride;ALPHA-[3-[[2-(3,4-DIMETHOXYPHENYL)ETHYL]METHYLAMINO]PROPYL]-3,4-DIMETHOXY-ALPHA-(1-METHYLETHYL)BENZENEACETONITRILE HYDROCHLORIDE;5-[(3,4-DIMETHOXYPHENETHYL)METHYLAMINO]-2-(3,4-DIMETHOXYPHENYL)-2-ISOPROPYL-VALERONITRILE HYDROCHLORIDE

CAS:23313-68-0

MF:C27H39ClN2O4

MW:491.06

EINECS:205-800-5

Product Categories:Intermediates & Fine Chemicals;Pharmaceuticals VERAPAMIL HYDROCHLORIDE

Chemical Properties: mp 142 C (dec.)(lit.) storage temp. 0-6C solubility methanol: 50 mg/mL, clear, colorless form powder color white

CAS DataBase Reference: 23313-68-0(

CAS DataBase Reference:) T,Xi Risk Statements 23/24/25-36/37/38 Safety Statements 36/37-45-37/39-26 RIDADR UN 2811 6.1/PG 3 WGK Germany 3 RTECS YV8320000 F 8-10 VERAPAMIL HYDROCHLORIDE

Usage And Synthesis:

Chemical Properties: White Powder UsageA calcium channel blocker. Antihypertensive; antianginal; antiarrhythmic (class IV) VERAPAMIL HYDROCHLORIDE



