



Formula: C<sub>27</sub>H<sub>39</sub>ClN<sub>2</sub>O<sub>4</sub>

MW: 491.07

CAS: 52-53-9

MDL: MFCD00055208

TNP: TNP00358



LogP: 4.51

LogS:

Acceptors: 4

Donors: 0

Rotation Bonds: 13

Chiral Centers: 1

N+O: 6

LIPINSKY: 4

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

ACTIVITY: Coronary vasodilator with calcium blocking activity

Merck 13 Reference: Monograph Number: 0010012

Title: Verapamil

CAS Registry Number: 52-53-9

CAS Name:

$\alpha$ -[3-[[2-(3,4-Dimethoxyphenyl)ethyl]methylamino]propyl]-3,4-dimethoxy- $\alpha$ -(1-methylethyl)benzene acetonitrile

Additional Names:

5-[(3,4-dimethoxyphenethyl)methylamino]-2-(3,4-dimethoxyphenyl)-2-isopropylvaleronitrile;  
 $\alpha$ -isopropyl- $\alpha$ -[(N-methyl-N-homoveratryl)- $\gamma$ -aminopropyl]-3,4-dimethoxyphenylacetonitrile;  
iproveratril

Manufacturers' Codes: D-365

Molecular Formula: C<sub>27</sub>H<sub>38</sub>N<sub>2</sub>O<sub>4</sub>

Molecular Weight: 454.60.

Percent Composition: C 71.33%, H 8.43%, N 6.16%, O 14.08%

Literature References: Prototype calcium antagonist; vasodilating activity resides primarily in the (S)-isomer. Both isomers inhibit the p-glycoprotein efflux pump in multidrug resistant tumor cells. Prepn: BE 615861; Dengel, US 3261859 (1962, 1966 both to Knoll). Pharmacology: H. Haas, G. H