VERAPAMIL

Other names:	5-((3,4-Dimethoxyphenethyl)methylamino)-2-(3,4-dimethoxyphenyl)-2-isopropylvaleronitri
	Benzeneacetonitrile, «alpha»-[3-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propyl]-3,4-dimethoxy-«alpha»-(1
	CP-16535-1
	D-365
	Dilacoran
	Iproveratril
	Valeronitrile, 5-((3,4-dimethoxyphenethyl)methylamino)-2-(3,4-dimethoxyphenyl)-2-isopropyl-
	Vasolan
	tryptamine
	«alpha»-((N-Methyl-N-homoveratryl)-«gamma»-aminopropyl)-3,4-dimethoxyphenylacetor
Inchi:	InChI=1S/C27H38N2O4/c1-20(2)27(19-28,22-10-12-24(31-5)26(18-22)33-7)14-8-15-29(3
InchiKey:	SGTNSNPWRIOYBX-UHFFFAOYSA-N
Formula:	C27H38N2O4
SMILES:	COc1ccc(CCN(C)CCCC(C#N)(c2ccc(OC)c(OC)c2)C(C)C)cc1OC
Mol. weight [g/mol]:	454.61

Physical Properties

Property code	Value	Unit	Source
hfus	50.55	kJ/mol	Joback Method
log10ws	-3.30		Aqueous Solubility Prediction Method
logp	5.093		Crippen Method
mcvol	378.610	ml/mol	McGowan Method
rinpol	3161.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
tf	439.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1288.74	J/mol×K	1090.97	Joback Method
cpg	1301.36	J/mol×K	1131.75	Joback Method
cpg	1312.12	J/mol×K	1172.53	Joback Method

cpg	1321.07	J/mol×K	1213.32	Joback Method
cpg	1328.27	J/mol×K	1254.10	Joback Method
cpg	1333.79	J/mol×K	1294.88	Joback Method
cpg	1337.68	J/mol×K	1335.66	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52539&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point