Ajmalicine

Other names:	Oxayohimban-16-carboxylic acid, 16,17-didehydro-19-methyl-, methyl ester, (19«alpha»)-
	«delta»-Yohimbine
	Ajmalicin
	Hydrosarpan
	Lamuran
	Py-tetrahydroserpentine
	Ranitol
	Raubaserp
	Raubasil
	Raubasin
	Raubasine
	Raumalina
	Rauvasan
	Sarpan
	Tensyl
	Tetrahydroserpentine
	Vincain
	Vincein
	Vinceine
	Alkaloid C
	Alkaloid F
	Alkaloid II
	Circolene
	Substance II
	16,17-Didehydro-19-methyloxayohimban-16-carboxylic acid methyl ester
	4H-Indolo[2,3-a]pyrano[3,4-g]quinolizine, oxayohimban-16-carboxylic acid deriv.
	16,17-Didehydro-19«alpha»-methyloxayohimban-16-carboxylic acid methyl ester
	Isoarteril
	(-)-Ajmalicin
	NSC 72133
Inchi:	InChI=1S/C21H24N2O3/c1-12-16-10-23-8-7-14-13-5-3-4-6-18(13)22-20(14)19(23)9-15(1
InchiKey:	GRTOGORTSDXSFK-UHFFFAOYSA-N
Formula:	C21H24N2O3
SMILES:	COC(=O)C1=COC(C)C2CN3CCc4c([nH]c5ccccc45)C3CC12
Mol. weight [g/mol]:	352.43
CAS:	483-04-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	2.697		Crippen Method
mcvol	264.220	ml/mol	McGowan Method
rinpol	3139.00		NIST Webbook
rinpol	3139.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C483045&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices