Methoserpidine

Other names: Yohimban-16-carboxylic acid, 10,17-dimethoxy-18-[(3,4,5-trimethoxybenzoyl)oxy]-, methyl ester, (3«beta»,16«beta»,17«alpha»,18«beta»,20«alpha»)-
(-)-10-Methoxydeserpidine
Canescine 10-methoxyderivative
Deaserpyl
Decaserpil
Decaserpin
Decaserpine
Decaserpyl
Decoserpyl
Deserpidine, 10-methoxy-
Minoran
Neoserpin
Resertene
Tenserpina
10-Methoxy-11-desmethoxyreserpine
10-MD
3«beta»,20«alpha»-Yohimban-16«beta»-carboxylic acid, 18«beta»-hydroxy-10,17«alpha»-dimethoxy-, methyl ester, 3,4,5-trimethoxybenzoate (ester)
3-«beta»-20-«alpha»-Yohimban-16-«beta»-carboxylic acid, 18-«beta»-hydroxy-10,17-«alpha»-dimethoxy-,methyl ester, 3,4,5-trimethoxybenzoate
Decaserpyl plus
R 694
10-Methoxydeserpidine
NSC 169423

Inchi: InChI=1S/C33H40N2O9/c1-38-19-7-8-23-22(14-19)20-9-10-35-16-18-13-27(44-32(36)17
InchiKey: ULBNWNUHGJLQHO-UHFFFAOYSA-N
Formula: C33H40N2O9
SMILES: COC(=O)C1C2CC3c4[nH]c5ccc(OC)cc5c4CCN3CC2CC(OC(=O)c2cc(OC)c(OC)c(OC)c2
Mol. weight [g/mol]: 608.68
CAS: 865-04-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	3.689		Crippen Method
mcvol	444.760	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C865043&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