

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»)- 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) 3,4,5-trimethoxybenzoate (ester) 18«beta»-hydroxy-10,17«alpha»-dimethoxy-,methyl ester, 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]:	608.69

Physical Properties

Property code	Value	Unit	Source
ie	7.12	eV	Cheméo Relay (1.0)
logp	3.689		Crippen Method
mcvol	444.760	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C865043&Units=SI

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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