

Deserpidine

Other names:	Yohimban-16-carboxylic acid, 17-methoxy-18-[(3,4,5-trimethoxybenzoyl)oxy]-, methyl ester, (3«beta»,16«beta»,17«alpha»,18«beta»,20«alpha»)-3«beta»,20«alpha»-Yohimban-16«beta»-carboxylic acid, 18«beta»-hydroxy-17«alpha»-methoxy-, methyl ester, 3,4,5-trimethoxybenzoate (ester) Canescin Canescine Deserpidin Harmonyl Raunormin Raunormine Recanescin Recanescine Reserpidine Reserpine, 11-demethoxy- 11-Demethoxyreserpine 11-Desmethoxyreserpine Benz(g)indolo(2,3-a)quinolizine-1-carboxylic acid, 1,2,3,4,4a,5,7,8,13,13b,14,14a-dodecahydro-3-hydroxy-2-methoxy-, methyl ester, 3,4,5-trimethoxybenzoate Deserpidine 3-«beta»,20-«alpha»-Yohimban-16-«beta»-carboxylic acid, 18-«beta»-hydroxy-17-«alpha»-methoxy-,methyl ester, 3,4,5-trimethoxybenzoate A-11025 Deresperine Desmethoxyreserpine LILLY 22641 Raunorine Tranquinil Methyl 17«alpha»-methoxy-18«beta»-[(3,4,5-trimethoxybenzoyl)oxy]-3«beta»,20«alpha»-yohimban-16«beta»-carboxylic acid, methyl ester Methyl 18«beta»-hydroxy-17«alpha»-methoxy-3«beta»,20«alpha»-yohimban-16«beta»-carboxylic acid, methyl ester NSC 72138 3,4,5-trimethoxybenzoate (ester) Deserpidic acid, methyl ester, 3,4,5-trimethoxybenzoate
Inchi:	InChI=1S/C32H38N2O8/c1-37-24-12-17(13-25(38-2)29(24)39-3)31(35)42-26-14-18-16-3
InchiKey:	CVBMAZKKCSYWQR-UHFFFAOYSA-N
Formula:	C32H38N2O8
SMILES:	COC(=O)C1C2CC3c4[nH]c5cccc5c4CCN3CC2CC(OC(=O)c2cc(OC)c(OC)c(OC)c2)C1
Mol. weight [g/mol]:	578.65
CAS:	131-01-1

Physical Properties

Property code	Value	Unit	Source
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log10ws	-6.28		Crippen Method
logp	3.681		Crippen Method
mcvol	424.800	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C131011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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