

SYROsingopine

Other names:	Yohimban-16-carboxylic acid, 18-[[4-[(ethoxycarbonyl)oxy]-3,5-dimethoxybenzoyl]oxy]-11,17-dimethoxy-, methyl ester, (3«beta»,16«beta»,17«alpha»,18«beta»,20«alpha»)- reserpate Carbethoxysyringoyl methylreserpate Elufinesin Etropres HF-41T Ipores Isotense Londomin Menatensina Methyl carbethoxysyringoyl reserpate Methyl reserpate ester of syringic acid ethyl carbonate Methyl reserpate, 4-ethoxycarbonyl-3,5-dimethoxybenzoic acid ester Neoreserpan Nichiserpine-S Novoserpina Raunova Reserpig acid, methyl ester, ester with 4-hydroxy-3,5-dimethoxybenzoic acid ethyl carbonate Revelox-Wirkstoff Seringina Serpagon Singoserp Siringal Siringina Siringone Siriserpin Siroshuten Su 3118 Syringic acid ethyl carbonate ester with methyl reserpate Syringopine Syroserpin Vegaserpina 3«beta»,20«alpha»-Yohimban-16«beta»-carboxylic acid, 18«beta»-hydroxy-11,17«alpha»-dimethoxy-, methyl ester, 3«beta»,20«alpha»-yohimban-16«beta»-carboxylic acid, 4-hydroxy-3,5-dimethoxybenzoate (ester) ethyl carbonate (ester) 18«beta»-hydroxy-11,17«alpha»-dimethoxy-, methyl ester, ester with 4-hydroxy-3,5-dimethoxybenzoic acid ethyl carbonate Methyl Sentramin acid methyl ester NSC 77030
Inchi:	InChI=1S/C35H42N2O11/c1-7-46-35(40)48-31-26(42-3)12-18(13-27(31)43-4)33(38)47-2
InchiKey:	ZCDNRPPFBQDQHR-UHFFFAOYSA-N

Formula: C35H42N2O11
SMILES: CCOC(=O)Oc1c(OC)cc(C(=O)OC2CC3CN4CCc5c([nH]c6cc(OC)ccc56)C4CC3C(C(=O)O)C2)cc1
Mol. weight [g/mol]: 666.72

Physical Properties

Property code	Value	Unit	Source
ie	7.20	eV	Cheméo Relay (1.0)
logp	4.216		Crippen Method
mcvol	480.380	ml/mol	McGowan Method

Sources

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=C84366&Units=SI>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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<https://www.chemeo.com/cid/97-170-6/SYROSINGOPINE.pdf>

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