Physostigmine

Other names:	Pyrrolo[2,3-b]indol-5-ol, 1,2,3,3a,8,8a-hexahydro-1,3a,8-trimethyl-, methylcarbamate (ester), (3aS-cis)-
	Eserine
	Esromiotin
	Ezerin
	Physostol
	Pyrrolo[2,3-b]indol-5-ol, 1,2,3,3a,8,8a-hexahydro-1,3a,8-trimethyl-, methylcarbamate, (3aS-cis)-
	Antilirium
	Carbamic acid, methyl-, ester with eseroline
	Erserine
	Eserolein, methylcarbamate (ester)
	CS 58525
	Eserolein, methylcarbamate
	Fysostigmin
	1,2,3,3a«beta»,8a«beta»-Hexahydro-1,3a,8-trimethylpyrrolo[2,3-b]-indol-5-yl methylcarbamate
	1,2,3,3a,8,8a-Hexahydro-1,3a,8-trimethylpyrrolo-[2,3-b]indol-5-yl methylcarbamate, (3aS-cis)-
	(3aS-cis)-1,2,3,3a,8,8a-Hexahydro-1,3a,8-trimethylpyrrolo[2,3-b]indol-5-olmethylcarbama
	Eserine (ester)
	(-)-Physostigmine
	MCV 4484
	NIH 10421
	NSC 30782
	Pyrrolo[2,3-b]indol-5-ol, 1,2,3,3a,8,8a-hexahydro-1,3a,8-trimethyl-, 5-(N-methylcarbamate), (3aS,8aR)-
Inchi:	InChI=1S/C15H21N3O2/c1-15-7-8-17(3)13(15)18(4)12-6-5-10(9-11(12)15)20-14(19)16-2
InchiKey:	PIJVFDBKTWXHHD-UHFFFAOYSA-N
Formula:	C15H21N3O2
SMILES:	CNC(=O)Oc1ccc2c(c1)C1(C)CCN(C)C1N2C
Mol. weight [g/mol]:	275.35
CAS:	57-47-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.774		Crippen Method
mcvol	214.110	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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