

Eseridine

Other names:	1,2-Oxazino[6,5-b]indol-6-ol, 2,3,4,4a,9,9a-hexahydro-2,4a,9-trimethyl-, methylcarbamate, (4aS-cis)- Eserine aminoxide Eserine oxide Geneserine 1,2-Oxazino(6,5-b)indol-6-ol, 2,3,4,4a,9,9a-hexahydro-2,4a,9-trimethyl-, methylcarbamate (ester), (4aS-cis)- (4aS,9aS)-2,3,4,4a,9,9a-Hexahydro-2,4a,9-trimethyl-1,2-oxazino[6,5-b]indol-6-ylmethylcarbamate Physostigmine aminoxide 2,4a,9-Trimethyl-2,3,4,4a,9,9a-hexahydro[1,2]oxazino[6,5-b]indol-6-yl methylcarbamate, (4aS-cis)- NSC 340071
Inchi:	InChI=1S/C15H21N3O3/c1-15-7-8-17(3)21-13(15)18(4)12-6-5-10(9-11(12)15)20-14(19)1
InchiKey:	CNBHDDDBNEKKMJH-UHFFFAOYSA-N
Formula:	C15H21N3O3
SMILES:	CNC(=O)Oc1ccc2c(c1)C1(C)CCN(C)OC1N2C
Mol. weight [g/mol]:	291.35
CAS:	25573-43-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	1.705		Crippen Method
mcvol	219.980	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=C25573437&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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