Spiro[2,5-cyclohexadiene-1,7'(1'H)-cyclopent[ij]isoquinoline-2',3',8',8'a-tetrahydro-5',6'-dimethoxy-1'-methyl-, (R)-

Other names:	Pronuciferine Milthanthine Pronuciferin N-Methylstepharine N,O-Dimethylcrotonosine (+)-Pronuciferine
Inchi:	InChI=1S/C19H21NO3/c1-20-9-6-12-10-15(22-2)18(23-3)17-16(12)14(20)11-19(17)7-4-1
InchiKey:	WUYQEGNOQLRQAQ-CQSZACIVSA-N
Formula:	C19H21NO3
SMILES:	COc1cc2c3c(c1OC)C1(C=CC(=O)C=C1)CC3N(C)CC2
Mol. weight [g/mol]:	311.37
CAS:	2128-60-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.569		Crippen Method
mcvol	236.920	ml/mol	McGowan Method
rinpol	2676.00		NIST Webbook
rinpol	2676.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2128601&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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