N-Methyllaurotetanine

Other names:	6a-«alpha»-Aporphin-9-ol, 1,2,10-trimethoxy- 4H-Dibenzo(de,g)quinolin-9-ol, 5,6,6a,7-tetrahydro-1,2,10-trimethoxy-6-methyl-, (S)- Lauroscholtzine (+)-N-Methyllaurotetanine Rogersine 1,2,10-Trimethoxy-6a-«alpha»-aporphin-9-ol
Inchi:	InChI=1S/C20H23NO4/c1-21-6-5-11-9-17(24-3)20(25-4)19-13-10-16(23-2)15(22)8-12(13
InchiKey:	ZFLRVRLYWHNAEC-UHFFFAOYSA-N
Formula:	C20H23NO4
SMILES:	COc1cc2c(cc1O)CC1c3c(cc(OC)c(OC)c3-2)CCN1C
Mol. weight [g/mol]:	341.40
CAS:	2169-44-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	3.170		Crippen Method
mcvol	256.880	ml/mol	McGowan Method
rinpol	2955.50		NIST Webbook
rinpol	2955.50		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2169440&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