

Furo[2,3-b]quinoline, 4,6,8-trimethoxy-

Other names:	Maculosidin Maculosidine Makulozidin 6,8-Dimethoxydictamnine
Inchi:	InChI=1S/C14H13NO4/c1-16-8-6-10-12(11(7-8)17-2)15-14-9(4-5-19-14)13(10)18-3/h4-7
InchiKey:	SHAVHFJCSQWTFF-UHFFFAOYSA-N
Formula:	C14H13NO4
SMILES:	COc1cc(OC)c2nc3occc3c(OC)c2c1
Mol. weight [g/mol]:	259.26
CAS:	522-19-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.94		Crippen Method
logp	3.007		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
rmpol	2471.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C522190&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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