OCTAVERINE

Other names:	Isoquinoline, 6,7-dimethoxy-1-(3,4,5-triethoxyphenyl)-
	6,7-Dimethoxy-1-(3,4,5-triethoxyphenyl)isoquinoline
	Oktaverine
	Octaverinum
Inchi:	InChI=1S/C23H27NO5/c1-6-27-20-12-16(13-21(28-7-2)23(20)29-8-3)22-17-14-19(26-5)1
InchiKey:	NGIFHAUKQGDVSR-UHFFFAOYSA-N
Formula:	C23H27NO5
SMILES:	CCOc1cc(-c2nccc3cc(OC)c(OC)cc23)cc(OCC)c1OCC
Mol. weight [g/mol]:	397.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Cheméo Relay (1.0)
logp	5.115		Crippen Method
mcvol	307.280	ml/mol	McGowan Method
tf	390.76	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C549688&Units=SI

Legend

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

tf: Normal melting (fusion) point

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