Moxaverine

Other names:	Isoquinoline, 3-ethyl-6,7-dimethoxy-1-(phenylmethyl)-
	1-Benzyl-3-ethyl-6,7-dimethoxyisoquinoline
	3-Ethyl-6,7-dimethoxy-1-(phenylmethyl)isoquinoline
	Isoquinoline, 1-benzyl-3-ethyl-6,7-dimethoxy
	Eupaverin
	3-Ethyl-1-benzyl-6,7-dimethoxyisoquinoline
Inchi:	InChI=1S/C20H21NO2/c1-4-16-11-15-12-19(22-2)20(23-3)13-17(15)18(21-16)10-14-8-6-
InchiKey:	MYCMTMIGRXJNSO-UHFFFAOYSA-N
Formula:	C20H21NO2
SMILES:	CCc1cc2cc(OC)c(OC)cc2c(Cc2ccccc2)n1
Mol. weight [g/mol]:	307.39
CAS:	10539-19-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.18		Crippen Method
logp	4.405		Crippen Method
mcvol	247.400	ml/mol	McGowan Method
rinpol	2518.00		NIST Webbook
rinpol	2488.00		NIST Webbook
rinpol	2518.00		NIST Webbook
rinpol	2488.00		NIST Webbook

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=C10539192&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
rinpol:	Non-polar retention indices