Mepixanthone

Other names:	mepixanox
Inchi:	InChI=1S/C20H21NO3/c1-23-17-10-9-15-19(22)14-7-3-4-8-18(14)24-20(15)16(17)13-21-
InchiKey:	PYSOHOOUXFWCFF-UHFFFAOYSA-N
Formula:	C20H21NO3
SMILES:	COc1ccc2c(=O)c3ccccc3oc2c1CN1CCCCC1
Mol. weight [g/mol]:	323.39
CAS:	17854-59-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.79		Crippen Method
logp	3.941		Crippen Method
mcvol	246.710	ml/mol	McGowan Method
rinpol	2799.00		NIST Webbook
rinpol	2799.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17854590&Units=SI

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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https://www.chemeo.com/cid/96-459-7/Mepixanthone.pdf

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