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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17854590&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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