Dimetacrine M(N-oxide)

Inchi: InChI=1S/C20H26N2O/c1-20(2)16-10-5-7-12-18(16)22(23,15-9-14-21(3)4)19-13-8-6-11-1
InchiKey: IBZAKFPEKZMOEJ-UHFFFAOYSA-N
Formula: C20H26N2O
SMILES: CN(C)CCC[N+]1([O-])c2ccccc2C(C)(C)c2ccccc21
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.20		Crippen Method
logp	4.414		Crippen Method
mcvol	260.110	ml/mol	McGowan Method
rinpol	2020.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R213108&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