perlapine

Inchi: InChI=1S/C19H21N3/c1-21-10-12-22(13-11-21)19-17-8-4-2-6-15(17)14-16-7-3-5-9-18(16
InchiKey: PWRPUAKXMQAFCJ-UHFFFAOYSA-N
Formula: C19H21N3
SMILES: CN1CCN(C2=Nc3ccccc3Cc3ccccc32)CC1
Mol. weight [g/mol]: 291.39
CAS: 1977-11-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	2.917		Crippen Method
mcvol	234.970	ml/mol	McGowan Method
rinpol	2421.00		NIST Webbook
rinpol	2421.00		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=C1977113&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