Zopiclone-N-oxide

Inchi: InChI=1S/C17H17ClN6O4/c1-22-6-8-23(9-7-22)17(26)28-16-14-13(19-4-5-20-14)15(25)2
InchiKey: DBSAMPORSYCNLC-UHFFFAOYSA-N
Formula: C17H17ClN6O4
SMILES: CN1CCN(C(=O)OC2c3nccnc3C(=O)[N+]2([O-])c2ccc(Cl)cn2)CC1
Mol. weight [g/mol]: 404.81

Physical Properties

Property code	Value	Unit	Source
log10ws	0.55		Crippen Method
logp	1.567		Crippen Method
mcvol	268.150	ml/mol	McGowan Method
rinpol	3050.00		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=R178520&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