mono-N-demethyladinazolam

Inchi: InChI=1S/C18H16ClN5/c1-20-10-16-22-23-17-11-21-18(12-5-3-2-4-6-12)14-9-13(19)7-8-
InchiKey: XPMACCNVZKHGPT-UHFFFAOYSA-N
Formula: C18H16ClN5
SMILES: CNCc1nnc2n1-c1ccc(Cl)cc1C(c1ccccc1)=NC2
Mol. weight [g/mol]: 337.81
CAS: 37115-33-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.97		Crippen Method
logp	2.991		Crippen Method
mcvol	244.480	ml/mol	McGowan Method
rinpol	3130.00		NIST Webbook
rinpol	3130.00		NIST Webbook

Sources

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=C37115336&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices