

Adinazolam

Inchi: InChI=1S/C19H18ClN5/c1-24(2)12-18-23-22-17-11-21-19(13-6-4-3-5-7-13)15-10-14(20)8
InchiKey: GJSLOMWRLALDCT-UHFFFAOYSA-N
Formula: C19H18ClN5
SMILES: CN(C)Cc1nnc2n1-c1ccc(Cl)cc1C(c1ccccc1)=NC2
Mol. weight [g/mol]: 351.83
CAS: 37115-32-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.77		Crippen Method
logp	3.333		Crippen Method
mcvol	258.570	ml/mol	McGowan Method
rinpol	3060.00		NIST Webbook
rinpol	3060.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C37115325&Units=SI>
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>

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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<https://www.chemeo.com/cid/91-867-9/Adinazolam.pdf>

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