

oxazolam, acetylated

Inchi: InChI=1S/C20H19CIN2O3/c1-13-11-22-12-19(25)23(14(2)24)18-9-8-16(21)10-17(18)20(21)
InchiKey: WGSUDUCAKBJSJF-XCLFUZPHSA-N
Formula: C20H19CIN2O3
SMILES: CC(=O)N1C(=O)CN2CC(C)OC2(c2ccccc2)c2cc(Cl)ccc21
Mol. weight [g/mol]: 370.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	3.155		Crippen Method
mcvol	264.630	ml/mol	McGowan Method
rinpole	2300.00		NIST Webbook
rinpole	2300.00		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=R325494&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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<https://www.chemeo.com/cid/117-002-9/oxazolam-acetylated.pdf>

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