

Oxazolam

Other names:	Oxazolo[3,2-d][1,4]benzodiazepin-6(5H)-one, 10-chloro-2,3,7,11b-tetrahydro-2-methyl-11b-phenyl- Benzo(6,7)-1,4-diazepino-(5,4-b)-oxazol-6-one, 10-chloro-2,3,5,6,7,11b-hexahydro-2-methyl-11b-phenyl- Oxazolazepam, Serenal 10-Chloro-2,3,7,11b-tetrahydro-2-methyl-11b-phenyloxazolo[3,2-d][1,4]benzodiazepin-6(5H)-one, Hializan Tranquit Serenal [Japanese]
Inchi:	InChI=1S/C18H17ClN2O2/c1-12-10-21-11-17(22)20-16-8-7-14(19)9-15(16)18(21,23-12)/h1-10,13-17,22-23H
InchiKey:	VCCZBYPHZRWKFY-UHFFFAOYSA-N
Formula:	C18H17ClN2O2
SMILES:	CC1CN2CC(=O)Nc3ccc(Cl)cc3C2(c2ccccc2)O1
Mol. weight [g/mol]:	328.79
CAS:	24143-17-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	3.214		Crippen Method
mcvol	234.880	ml/mol	McGowan Method
rinpol	2564.00		NIST Webbook
rinpol	2569.00		NIST Webbook
rinpol	2586.00		NIST Webbook
rinpol	2596.00		NIST Webbook
rinpol	2590.00		NIST Webbook
rinpol	2564.00		NIST Webbook
rinpol	2590.00		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=C24143177&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

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