Zopiclone

Other names:	1-Piperazinecarboxylic acid, 4-methyl-, 6-(5-chloro-2-pyridinyl)-6,7-dihydro-7-oxo-5H-pyrrolo[3,4-b]pyrazin-5-yl ester
	Amoban
	Amovane
	Imovane
	27267 R.P.
	4-Methyl-1-piperazinecarboxylic acid ester with 6-(5-chloro-2-pyridyl)-6,7-dihydro-7-hydroxy-5H-pyrrolo[3,4-b]pyrazin-5-one
	Imovance
	RP-27267
	Sopivan
	Zimovane
	(.+/-.)-Zopiclone
Inchi:	InChI=1S/C17H17ClN6O3/c1-22-6-8-23(9-7-22)17(26)27-16-14-13(19-4-5-20-14)15(25)2
InchiKey:	GBBSUAFBMRNDJC-UHFFFAOYSA-N
Formula:	C17H17ClN6O3
SMILES:	CN1CCN(C(=O)OC2c3nccnc3C(=O)N2c2ccc(Cl)cn2)CC1
Mol. weight [g/mol]:	388.81
CAS:	43200-80-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	1.568		Crippen Method
mcvol	262.280	ml/mol	McGowan Method
rinpol	3051.00		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=C43200802&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

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https://www.chemeo.com/cid/47-135-0/Zopiclone.pdf

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