

Zopiclone-M/artifact (amino-chloro-pyridine) AC

Inchi:	InChI=1S/C7H7ClN2O/c1-5(11)10-7-3-2-6(8)4-9-7/h2-4H,1H3,(H,9,10,11)
InchiKey:	MCCVKQDZALWIQD-UHFFFAOYSA-N
Formula:	C7H7ClN2O
SMILES:	CC(=O)Nc1ccc(Cl)cn1
Mol. weight [g/mol]:	170.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	1.693		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
rinsol	1505.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinsol:	Non-polar retention indices

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