

Zopiclone-M/artifact (alcohol) AC

Inchi: InChI=1S/C13H9CIN4O3/c1-7(19)21-13-11-10(15-4-5-16-11)12(20)18(13)9-3-2-8(14)6-1
InchiKey: CDKPEDZDDURJIN-UHFFFAOYSA-N
Formula: C13H9CIN4O3
SMILES: CC(=O)OC1c2nccnc2C(=O)N1c1ccc(Cl)cn1
Mol. weight [g/mol]: 304.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	1.747		Crippen Method
mcvol	196.820	ml/mol	McGowan Method
rinpol	2390.00		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=R331296&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/33-674-7/Zopiclone-M-artifact-alcohol-AC.pdf>

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