

«alpha»-hydroxy-alprazolam

Inchi: InChI=1S/C17H13ClN4O/c18-12-6-7-14-13(8-12)17(11-4-2-1-3-5-11)19-9-15-20-21-16(1)
InchiKey: ZURUZYHEEMDQBU-UHFFFAOYSA-N
Formula: C17H13ClN4O
SMILES: OCc1nnc2n1-c1ccc(Cl)cc1C(c1ccccc1)=NC2
Mol. weight [g/mol]: 324.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.62		Crippen Method
logp	2.764		Crippen Method
mcvol	226.280	ml/mol	McGowan Method
rinpol	3010.00		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=R84954&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/57-190-8/alpha-hydroxy-alprazolam.pdf>

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