

«alpha»-hydroxy-triazolam

Inchi: InChI=1S/C17H12Cl2N4O/c18-10-5-6-14-12(7-10)17(11-3-1-2-4-13(11)19)20-8-15-21-22
InchiKey: BHUYWUDMVCLHND-UHFFFAOYSA-N
Formula: C17H12Cl2N4O
SMILES: OCC1nnc2n1-c1ccc(Cl)cc1C(c1ccccc1Cl)=NC2
Mol. weight [g/mol]: 359.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.31		Crippen Method
logp	3.417		Crippen Method
mcvol	238.520	ml/mol	McGowan Method
rinpola	3020.00		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=R84968&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/11-848-8/alpha-hydroxy-triazolam.pdf>

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