

3-Hydroxyprazepam

Inchi: InChI=1S/C18H15ClN2O2/c19-12-6-9-15-14(10-12)16(11-4-2-1-3-5-11)20-17(22)18(23)2
InchiKey: FSBZZQYOKRMUSO-UHFFFAOYSA-N
Formula: C18H15ClN2O2
SMILES: O=C1C(O)N=C(c2ccccc2)c2cc(Cl)ccc2N1C1CC1
Mol. weight [g/mol]: 326.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	3.005		Crippen Method
mcvol	230.580	ml/mol	McGowan Method
rinpol	2860.00		NIST Webbook
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Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R17391&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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