

3-hydroxy-2-oxoquazepam

Inchi: InChI=1S/C17H11ClF4N2O2/c18-9-5-6-13-11(7-9)14(10-3-1-2-4-12(10)19)23-15(25)16(2)
InchiKey: UUODKRKSEPDUBO-UHFFFAOYSA-N
Formula: C17H11ClF4N2O2
SMILES: O=C1C(O)N=C(c2ccccc2F)c2cc(Cl)ccc2N1CC(F)(F)F
Mol. weight [g/mol]: 386.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.80		Crippen Method
logp	3.544		Crippen Method
mcvol	234.430	ml/mol	McGowan Method
rinpol	2405.00		NIST Webbook
rinpol	2405.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R522264&Units=SI>

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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