

7-Aminoflunitrazepam

Inchi: InChI=1S/C16H14FN3O/c1-20-14-7-6-10(18)8-12(14)16(19-9-15(20)21)11-4-2-3-5-13(11)
InchiKey: LTCDLGUFORGHGY-UHFFFAOYSA-N
Formula: C16H14FN3O
SMILES: CN1C(=O)CN=C(c2ccccc2F)c2cc(N)ccc21
Mol. weight [g/mol]: 283.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	2.222		Crippen Method
mcvol	206.900	ml/mol	McGowan Method
rinpol	2725.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2723.00		NIST Webbook
rinpol	2726.00		NIST Webbook
rinpol	2726.00		NIST Webbook
rinpol	2719.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R17074&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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