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
CAS: 34084-50-9

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	2745.00		NIST Webbook
rinpol	2745.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C34084509&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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