

7-Acetamidoflunitrazepam

Inchi: InChI=1S/C18H16FN3O2/c1-11(23)21-12-7-8-16-14(9-12)18(20-10-17(24)22(16)2)13-5-3
InchiKey: MMTDAQLJAWIUTN-UHFFFAOYSA-N
Formula: C18H16FN3O2
SMILES: CC(=O)Nc1ccc2c(c1)C(c1ccccc1F)=NCC(=O)N2C
Mol. weight [g/mol]: 325.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	2.598		Crippen Method
mcvol	236.650	ml/mol	McGowan Method
rinpole	3115.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R17426&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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