

Tryptamine, 1-PFP

Inchi: InChI=1S/C13H11F5N2O/c14-12(15,13(16,17)18)11(21)19-6-5-8-7-20-10-4-2-1-3-9(8)10
InchiKey: VGGYHGSBLATFTE-UHFFFAOYSA-N
Formula: C13H11F5N2O
SMILES: O=C(NCCc1c[nH]c2ccccc12)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 306.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	2.542		Crippen Method
mcvol	185.490	ml/mol	McGowan Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		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=R580062&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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