

5-Hydroxytryptamine, methyl, 2-PFP

Inchi: InChI=1S/C17H12F10N2O3/c1-28(12(31)14(18,19)16(22,23)24)5-4-8-7-29(11-3-2-9(30)6)
InchiKey: BDESVKGIYFTGJB-UHFFFAOYSA-N
Formula: C17H12F10N2O3
SMILES: CN(CCc1cn(C(=O)C(F)(F)C(F)(F)F)c2ccc(O)cc12)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 482.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.14		Crippen Method
logp	4.383		Crippen Method
mcvol	258.140	ml/mol	McGowan Method
rinpol	2029.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580017&Units=SI>
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>

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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