5-Hydroxytryptophan, methyl, 2-PFP

Inchi: InChI=1S/C19H14F10N2O5/c1-30(14(34)16(20,21)18(24,25)26)12(13(33)36-2)5-8-7-31(
InchiKey: ZDHDCRAOTJITHN-UHFFFAOYSA-N
Formula: C19H14F10N2O5
SMILES: COC(=O)C(Cc1cn(C(=O)C(F)(F)C(F)(F)F)c2ccc(O)cc12)N(C)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 540.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.95		Crippen Method
logp	3.925		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
rinpol	2161.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R580022&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices