

5-Hydroxyindoleacetic acid, methyl, 1-PFP

Inchi: InChI=1S/C14H10F5NO4/c1-24-11(22)4-7-6-20(10-3-2-8(21)5-9(7)10)12(23)13(15,16)14
InchiKey: ZONBYMAMSQKAJQ-UHFFFAOYSA-N
Formula: C14H10F5NO4
SMILES: COC(=O)Cc1cn(C(=O)C(F)(F)C(F)(F)F)c2ccc(O)cc12
Mol. weight [g/mol]: 351.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Crippen Method
logp	2.900		Crippen Method
mcvol	202.910	ml/mol	McGowan Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R579983&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
rinpol: Non-polar retention indices

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