

Tryptamine, 2-PFP

Inchi: InChI=1S/C16H10F10N2O2/c17-13(18,15(21,22)23)11(29)27-6-5-8-7-28(10-4-2-1-3-9(8))
InchiKey: IARKHWXWSFQUKZ-UHFFFAOYSA-N
Formula: C16H10F10N2O2
SMILES: O=C(NCCc1cn(C(=O)C(F)(F)C(F)(F)F)c2ccccc12)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 452.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.79		Crippen Method
logp	4.335		Crippen Method
mcvol	238.180	ml/mol	McGowan Method
rinpola	1755.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.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=R580077&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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<https://www.chemeo.com/cid/58-896-4/Tryptamine-2-PFP.pdf>

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