

Fluacrypprim

Inchi: InChI=1S/C20H21F3N2O5/c1-12(2)30-19-24-16(20(21,22)23)9-17(25-19)29-10-13-7-5-6
InchiKey: MXWAGQASUDSFBG-RVDMUPIBSA-N
Formula: C20H21F3N2O5
SMILES: COC=C(C(=O)OC)c1ccccc1COc1cc(C(F)(F)F)nc(OC(C)C)n1
Mol. weight [g/mol]: 426.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.93		Crippen Method
logp	4.022		Crippen Method
mcvol	291.160	ml/mol	McGowan Method
rinpola	2289.00		NIST Webbook
rinpola	2289.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R566526&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/123-473-0/Fluacrypprim.pdf>

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