

Merresectine E

Inchi: InChI=1S/C20H27NO3/c1-13(2)4-5-14-10-15(6-9-19(14)22)20(23)24-18-11-16-7-8-17(12)
InchiKey: WDYARZUQOMDODE-PIIMJCKOSA-N
Formula: C20H27NO3
SMILES: CC(C)=CCc1cc(C(=O)OC2CC3CCC(C2)N3C)ccc1O
Mol. weight [g/mol]: 329.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.80		Crippen Method
logp	3.683		Crippen Method
mcvol	266.170	ml/mol	McGowan Method
rinpola	2685.00		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=R510093&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/48-390-6/Merresectine-E.pdf>

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