

3«beta»-Merresectine D

Inchi: InChI=1S/C21H29NO4/c1-13(2)5-6-14-9-15(10-19(25-4)20(14)23)21(24)26-18-11-16-7-8
InchiKey: ONGAXCZYCQUMSY-BCDXTJNWSA-N
Formula: C21H29NO4
SMILES: COc1cc(C(=O)OC2CC3CCC(C2)N3C)cc(CC=C(C)C)c1O
Mol. weight [g/mol]: 359.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	3.691		Crippen Method
mcvol	286.130	ml/mol	McGowan Method
rinpole	2813.00		NIST Webbook
rinpole	2813.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R509687&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpole: Non-polar retention indices

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