

3«beta»-(4-Hydroxybenzoyloxy)tropane

Inchi: InChI=1S/C15H19NO3/c1-16-11-4-5-12(16)9-14(8-11)19-15(18)10-2-6-13(17)7-3-10/h2-3
InchiKey: VXNQEEYJSNEORM-UHFFFAOYSA-N
Formula: C15H19NO3
SMILES: CN1C2CCC1CC(OC(=O)c1ccc(O)cc1)C2
Mol. weight [g/mol]: 261.32
CAS: 198898-04-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	2.174		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
rinpol	2282.00		NIST Webbook
rinpol	2369.00		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=C198898043&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
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/77-083-5/3-beta-4-Hydroxybenzoyloxy-tropane.pdf>

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