

Nootkatin

Inchi: InChI=1S/C15H20O2/c1-10(2)5-6-12-7-8-14(16)15(17)9-13(12)11(3)4/h5,7-9,11H,6H2,1-
InchiKey: MNMNTZYOZZLKSV-UHFFFAOYSA-N
Formula: C15H20O2
SMILES: CC(C)=CCc1ccc(O)c(=O)cc1C(C)C
Mol. weight [g/mol]: 232.32
CAS: 4431-03-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	3.384		Crippen Method
mcvol	201.590	ml/mol	McGowan Method
rinpol	1961.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4431032&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/92-971-2/Nootkatin.pdf>

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