

3-(2'-Hydroxytropoyloxy)-tropane

Inchi: InChI=1S/C17H23NO4/c1-18-13-7-8-14(18)10-15(9-13)22-16(20)17(21,11-19)12-5-3-2-4
InchiKey: LNAGCMLWANGVDE-KWOWKCNFSA-N
Formula: C17H23NO4
SMILES: CN1C2CCC1CC(OC(=O)C(O)(CO)c1ccccc1)C2
Mol. weight [g/mol]: 305.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	1.035		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
rinpole	2284.00		NIST Webbook
rinpole	2284.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R421319&Units=SI>

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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