

Supinine

Inchi: InChI=1S/C15H25NO4/c1-10(2)15(19,11(3)17)14(18)20-9-12-7-13-5-4-6-16(13)8-12/h8,10-14,16-18,20-21/t15,19,20,21
InchiKey: APQQKMAYNOGMPK-LKVSRLFHLSA-N
Formula: C15H25NO4
SMILES: CC(C)C(O)(C(=O)OCC1=CN2CCCC2C1)C(C)O
Mol. weight [g/mol]: 283.36
CAS: 551-58-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	1.049		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
rinpol	1977.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=C551586&Units=SI>

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/53-005-7/Supinine.pdf>

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