

trachelanthamine

Inchi: InChI=1S/C15H27NO4/c1-10(2)15(19,11(3)17)14(18)20-9-12-6-8-16-7-4-5-13(12)16/h10
InchiKey: BWQSLRZZOVFVHJ-FLTXBFBQSA-N
Formula: C15H27NO4
SMILES: CC(C)C(O)(C(=O)OCC1CCN2CCCC12)C(C)O
Mol. weight [g/mol]: 285.38
CAS: 14140-18-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Crippen Method
logp	0.782		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
rinpol	1970.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1965.00		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=C14140182&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/62-083-1/trachelanthamine.pdf>

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