

cis-adenocarpine

Inchi: InChI=1S/C19H26N2O/c22-19(12-11-16-7-2-1-3-8-16)21-14-6-9-17(15-21)18-10-4-5-13-
InchiKey: XIZYLQMCWHMQNP-QXMHVHEDSA-N
Formula: C19H26N2O
SMILES: O=C(C=Cc1cccc1)N1CCCC(C2CCCCN2)C1
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.09		Crippen Method
logp	3.081		Crippen Method
mcvol	250.320	ml/mol	McGowan Method
rinsol	2530.00		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=R317681&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
rinsol: Non-polar retention indices

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<https://www.chemeo.com/cid/37-089-3/cis-adenocarpine.pdf>

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