

# trans-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-VAWYXSNFSA-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
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R317696&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## 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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