

# Carnegine

**Other names:**

Isoquinoline, 1,2,3,4-tetrahydro-6,7-dimethoxy-1,2-dimethyl-, (.+/-.)-  
Carnegin  
Pectenin  
Pectenine

Isoquinoline, 1,2,3,4-tetrahydro-6,7-dimethoxy-1,2-dimethyl-, ( $\pm$ )-  
(+/-)-Pectenine

**Inchi:**

InChI=1S/C13H19NO2/c1-9-11-8-13(16-4)12(15-3)7-10(11)5-6-14(9)2/h7-9H,5-6H2,1-4H

**InchiKey:**

HRSIPKSSEVRSPG-UHFFFAOYSA-N

**Formula:**

C13H19NO2

**SMILES:**

COc1cc2c(cc1OC)C(C)N(C)CC2

**Mol. weight [g/mol]:**

221.30

**CAS:**

490-53-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.253		Crippen Method
mvol	181.130	ml/mol	McGowan Method
rmpol	1727.00		NIST Webbook
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## Sources

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C490539&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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