

# Isoangustifoline

**Inchi:** InChI=1S/C14H22N2O/c1-2-3-13-12-6-10(8-15-13)9-16-5-4-11(17)7-14(12)16/h2,10,12-14  
**InchiKey:** SHZTWMVOBAEJMJ-UHFFFAOYSA-N  
**Formula:** C14H22N2O  
**SMILES:** C=CCC1NCC2CC1C1CC(=O)CCN1C2  
**Mol. weight [g/mol]:** 234.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	1.204		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
rinpol	2051.00		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	2033.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R205439&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

Latest version available from:

<https://www.cheméo.com/cid/48-177-3/Isoangustifoline.pdf>

Generated by Cheméo on 2024-04-18 14:45:04.643189268 +0000 UTC m=+15740753.563766585.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.