

# Lusitanine

**Inchi:** InChI=1S/C12H20N2O/c1-10(15)13-9-11-5-4-8-14-7-3-2-6-12(11)14/h9,12H,2-8H2,1H3,  
**InchiKey:** XKKRQPPGOROKBD-PKNBQFBNSA-N  
**Formula:** C12H20N2O  
**SMILES:** CC(=O)NC=C1CCCN2CCCCC12  
**Mol. weight [g/mol]:** 208.30  
**CAS:** 5121-36-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	1.655		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1880.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5121368&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.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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