

# Sophoramine

**Inchi:** InChI=1S/C15H20N2O/c18-14-7-1-6-13-12-5-3-9-16-8-2-4-11(15(12)16)10-17(13)14/h1,6  
**InchiKey:** MMCQRJPAMIHQX-UHFFFAOYSA-N  
**Formula:** C15H20N2O  
**SMILES:** O=C1CCCC2N1CC1CCCN3CCCC2C13  
**Mol. weight [g/mol]:** 244.33  
**CAS:** 6882-66-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.820		Crippen Method
mcvol	191.700	ml/mol	McGowan Method
rinpole	2274.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=C6882662&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpole:** Non-polar retention indices

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