

# 1-(Piperidin-1-yl)hexadecan-1-one

**Inchi:** InChI=1S/C21H41NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-15-18-21(23)22-19-16-14-17-20-2  
**InchiKey:** SBWUACYNOBUPAH-UHFFFAOYSA-N  
**Formula:** C21H41NO  
**SMILES:** CCCCCCCCCCCCCCCC(=O)N1CCCCC1  
**Mol. weight [g/mol]:** 323.56  
**CAS:** 4629-02-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.85		Crippen Method
logp	6.480		Crippen Method
mcvol	307.440	ml/mol	McGowan Method
rinpol	2634.20		NIST Webbook
rinpol	2606.00		NIST Webbook
rinpol	2606.00		NIST Webbook
rinpol	2634.20		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4629021&Units=SI>  
**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)

## 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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