

# (2E,4E)-1-(Pyrrolidin-1-yl)tetradeca-2,4-dien-1-one

**Inchi:** InChI=1S/C18H31NO/c1-2-3-4-5-6-7-8-9-10-11-12-15-18(20)19-16-13-14-17-19/h10-12,15,18,20  
**InchiKey:** NYLFQLXBQJZGOR-GCHFJXRNSA-N  
**Formula:** C18H31NO  
**SMILES:** CCCCCCCCCC=CC=CC(=O)N1CCCC1  
**Mol. weight [g/mol]:** 277.44  
**CAS:** 88855-41-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	4.862		Crippen Method
mcvol	256.570	ml/mol	McGowan Method
rinpole	2562.10		NIST Webbook
rinpole	2562.10		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=C88855418&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

Latest version available from:

<https://www.chemeo.com/cid/81-918-3/2E-4E-1-Pyrrolidin-1-yl-tetradeca-2-4-dien-1-one.pdf>

Generated by Cheméo on 2024-04-23 12:21:46.475869241 +0000 UTC m=+16164155.396446557.  
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.