

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

**Inchi:** InChI=1S/C16H27NO/c1-2-3-4-5-6-7-8-9-10-13-16(18)17-14-11-12-15-17/h8-10,13H,2-7  
**InchiKey:** UAIYHWLHQSKQLW-PEGOPYGQSA-N  
**Formula:** C16H27NO  
**SMILES:** CCCCCC=CC=CC(=O)N1CCCC1  
**Mol. weight [g/mol]:** 249.39  
**CAS:** 117137-69-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	4.082		Crippen Method
mcvol	228.390	ml/mol	McGowan Method
rinpol	2346.50		NIST Webbook
rinpol	2323.00		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=C117137696&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

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