

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

**Inchi:** InChI=1S/C22H39NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22(24)23-20-17-18-2  
**InchiKey:** AVSSMWIINDFJMN-VNXILKCPSA-N  
**Formula:** C22H39NO  
**SMILES:** CCCCCCCCCCCCCC=CC=CC(=O)N1CCCC1  
**Mol. weight [g/mol]:** 333.55  
**CAS:** 102934-33-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.98		Crippen Method
logp	6.422		Crippen Method
mcvol	312.930	ml/mol	McGowan Method
rinpol	2996.80		NIST Webbook
rinpol	2996.80		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=C102934338&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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