

# (2E,4E,12E)-1-(Piperidin-1-yl)octadeca-2,4,12-trien-1-one

**Inchi:** InChI=1S/C23H39NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-23(25)24-21-18-16-15  
**InchiKey:** HFWMTBWJCPVZTO-NMPGFTJCSA-N  
**Formula:** C23H39NO  
**SMILES:** CCCCCC=CCCCCCCC=CC=CC(=O)N1CCCCC1  
**Mol. weight [g/mol]:** 345.56  
**CAS:** 943546-19-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.25		Crippen Method
logp	6.588		Crippen Method
mcvol	322.720	ml/mol	McGowan Method
rinpol	3014.80		NIST Webbook
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## Sources

**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=C943546198&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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