

# (9Z,11E)-Hexadeca-9,11-dien-1-ol, adduct with 4-methyl-3,5-dihydro-1,2,4-triazole-3,5-dione

**Inchi:** InChI=1S/C19H33N3O3/c1-3-4-11-16-13-14-17(12-9-7-5-6-8-10-15-23)22-19(25)20(2)18  
**InchiKey:** GIGHUEGEVMIZMA-UHFFFAOYSA-N  
**Formula:** C19H33N3O3  
**SMILES:** CCCCC1C=CC(CCCCCCCO)n2c(=O)n(C)c(=O)n21  
**Mol. weight [g/mol]:** 351.48

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.09		Crippen Method
logp	2.914		Crippen Method
mcvol	291.500	ml/mol	McGowan Method
rinpol	1842.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1842.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R558753&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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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