

# 1-Thiacyclodeca-3,8-diyne

**Inchi:** InChI=1S/C9H10S/c1-2-4-6-8-10-9-7-5-3-1/h1-3,8-9H2  
**InchiKey:** BIXURTSOTIYEDE-UHFFFAOYSA-N  
**Formula:** C9H10S  
**SMILES:** C1#CCSCC#CCCC1  
**Mol. weight [g/mol]:** 150.24  
**CAS:** 115227-74-2

## Physical Properties

Property code	Value	Unit	Source
ie	8.10	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
log10ws	-2.96		Crippen Method
logp	1.910		Crippen Method
mcvol	125.960	ml/mol	McGowan Method

## 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=C115227742&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**ie:** Ionization energy  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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