

# 1,8-Cyclopentadecadiyne

<b>Inchi:</b>	InChI=1S/C15H22/c1-2-4-6-8-10-12-14-15-13-11-9-7-5-3-1/h1-6,11-15H2
<b>InchiKey:</b>	LLYOCFZRRCOXMHY-UHFFFAOYSA-N
<b>Formula:</b>	C15H22
<b>SMILES:</b>	C1#CCCCCCCC#CCCCC1
<b>Mol. weight [g/mol]:</b>	202.34
<b>CAS:</b>	4722-42-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.59		Crippen Method
logp	4.298		Crippen Method
mcpvol	194.150	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.00 ± 5.00	K	0.00	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4722423&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4722423&amp;Units=SI</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**tbrp:** Boiling point at reduced pressure

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