

# 1,1,4,4-Tetramethylcyclododec-8-yne

<b>Inchi:</b>	InChI=1S/C16H28/c1-15(2)11-9-7-5-6-8-10-12-16(3,4)14-13-15/h7-14H2,1-4H3
<b>InchiKey:</b>	JWMCSWXRLWAYIJ-UHFFFAOYSA-N
<b>Formula:</b>	C16H28
<b>SMILES:</b>	CC1(C)CCCC#CCCC(C)(C)CC1
<b>Mol. weight [g/mol]:</b>	220.39
<b>CAS:</b>	15753-76-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.73		Crippen Method
logp	5.177		Crippen Method
mcvol	216.840	ml/mol	McGowan Method

## Sources

<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=C15753761&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15753761&amp;Units=SI</a>
<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>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/46-269-3/1-1-4-4-Tetramethylcyclododec-8-yne.pdf>

Generated by Cheméo on 2024-04-30 01:14:40.261712912 +0000 UTC m=+16728929.182290227.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.