

# 4-Hexadecen-6-yne, (E)-

<b>Inchi:</b>	InChI=1S/C16H28/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h7,9H,3-6,8,10,12,14-16H2,
<b>InchiKey:</b>	XZDCEQPWFZIZPQ-VQHVLOKHS-A-N
<b>Formula:</b>	C16H28
<b>SMILES:</b>	CCCC=CC#CCCCCCCCC
<b>Mol. weight [g/mol]:</b>	220.39
<b>CAS:</b>	74744-51-7

## Physical Properties

Property code	Value	Unit	Source
gf	366.86	kJ/mol	Joback Method
hf	15.95	kJ/mol	Joback Method
hfus	40.52	kJ/mol	Joback Method
hvap	53.32	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.487		Crippen Method
mvol	223.400	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
tb	578.64	K	Joback Method
tc	760.02	K	Joback Method
tf	371.10	K	Joback Method
vc	0.874	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.53	J/mol×K	578.64	Joback Method
cpg	576.15	J/mol×K	608.87	Joback Method
cpg	593.93	J/mol×K	639.10	Joback Method
cpg	610.90	J/mol×K	669.33	Joback Method
cpg	627.09	J/mol×K	699.56	Joback Method
cpg	642.53	J/mol×K	729.79	Joback Method
cpg	657.27	J/mol×K	760.02	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C74744517&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C74744517&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/74-082-9/4-Hexadecen-6-yne-E.pdf>

Generated by Cheméo on 2024-04-30 17:43:55.379601547 +0000 UTC m=+16788284.300178862.

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