

# 1,6-Octadiyne

Inchi:	InChI=1S/C8H10/c1-3-5-7-8-6-4-2/h1H,5,7-8H2,2H3
InchiKey:	HUPKWBBKMAGWFY-UHFFFAOYSA-N
Formula:	C8H10
SMILES:	C#CCCCCC#CC
Mol. weight [g/mol]:	106.17

## Physical Properties

Property code	Value	Unit	Source
gf	442.35	kJ/mol	Joback Method
hf	355.75	kJ/mol	Joback Method
hfus	22.57	kJ/mol	Joback Method
hvap	35.41	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.813		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpola	825.00		NIST Webbook
tb	381.56	K	Joback Method
tc	583.07	K	Joback Method
tf	332.99	K	Joback Method
vc	0.407	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.04	J/mol×K	381.56	Joback Method
cpg	194.38	J/mol×K	415.15	Joback Method
cpg	204.23	J/mol×K	448.73	Joback Method
cpg	213.62	J/mol×K	482.32	Joback Method
cpg	222.57	J/mol×K	515.90	Joback Method
cpg	231.08	J/mol×K	549.49	Joback Method
cpg	239.19	J/mol×K	583.07	Joback Method

# Sources

<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=R144804&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R144804&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>

# 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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<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/55-704-9/1-6-Octadiyne.pdf>

Generated by Cheméo on 2024-04-23 15:03:00.955298848 +0000 UTC m=+16173829.875876163.

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