

# 4-Nonen-2-yne, (E)-

<b>Other names:</b>	Non-2-yn-4-ene, (E)-
<b>Inchi:</b>	InChI=1S/C9H14/c1-3-5-7-9-8-6-4-2/h8-9H,3,5,7H2,1-2H3/b9-8+
<b>InchiKey:</b>	AIDMRHRNBMILQM-CMDGGGOBGSA-N
<b>Formula:</b>	C9H14
<b>SMILES:</b>	CC#CC=CCCC
<b>Mol. weight [g/mol]:</b>	122.21
<b>CAS:</b>	53497-79-3

## Physical Properties

Property code	Value	Unit	Source
gf	307.92	kJ/mol	Joback Method
hf	160.43	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hvap	37.74	kJ/mol	Joback Method
ie	8.46 ± 0.01	eV	NIST Webbook
log10ws	-3.24		Crippen Method
logp	2.756		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	418.48	K	Joback Method
tc	614.03	K	Joback Method
tf	292.21	K	Joback Method
vc	0.481	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.02	J/molxK	418.48	Joback Method
cpg	245.08	J/molxK	451.07	Joback Method
cpg	257.51	J/molxK	483.66	Joback Method
cpg	269.36	J/molxK	516.26	Joback Method
cpg	280.63	J/molxK	548.85	Joback Method
cpg	291.36	J/molxK	581.44	Joback Method
cpg	301.57	J/molxK	614.03	Joback 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>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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C53497793&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53497793&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>ie:</b>	Ionization energy
<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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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