

# 1-Chloro-4-nonyne

<b>Inchi:</b>	InChI=1S/C9H15Cl/c1-2-3-4-5-6-7-8-9-10/h2-4,7-9H2,1H3
<b>InchiKey:</b>	RHZYERSKMQJUCP-UHFFFAOYSA-N
<b>Formula:</b>	C9H15Cl
<b>SMILES:</b>	CCCCC#CCCCCl
<b>Mol. weight [g/mol]:</b>	158.67
<b>CAS:</b>	3416-74-8

## Physical Properties

Property code	Value	Unit	Source
gf	215.77	kJ/mol	Joback Method
hf	27.47	kJ/mol	Joback Method
hfus	26.39	kJ/mol	Joback Method
hvap	42.16	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.199		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	451.75	K	Joback Method
tc	644.56	K	Joback Method
tf	327.21	K	Joback Method
vc	0.550	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.84	J/mol×K	451.75	Joback Method
cpg	288.77	J/mol×K	483.88	Joback Method
cpg	301.13	J/mol×K	516.02	Joback Method
cpg	312.95	J/mol×K	548.15	Joback Method
cpg	324.24	J/mol×K	580.29	Joback Method
cpg	335.01	J/mol×K	612.42	Joback Method
cpg	345.29	J/mol×K	644.56	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.00	K	5.30	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>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=C3416748&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3416748&amp;Units=SI</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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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