

# 1-Pentyne, 3-chloro-4-methyl

<b>Inchi:</b>	InChI=1S/C6H9Cl/c1-4-6(7)5(2)3/h1,5-6H,2-3H3
<b>InchiKey:</b>	UVURCMLRAYOFEK-UHFFFAOYSA-N
<b>Formula:</b>	C6H9Cl
<b>SMILES:</b>	C#CC(Cl)C(C)C
<b>Mol. weight [g/mol]:</b>	116.59

## Physical Properties

Property code	Value	Unit	Source
gf	205.90	kJ/mol	Joback Method
hf	98.43	kJ/mol	Joback Method
hfus	11.42	kJ/mol	Joback Method
hvap	32.42	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.883		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
rinpola	754.00		NIST Webbook
tb	363.35	K	Joback Method
tc	557.52	K	Joback Method
tf	204.27	K	Joback Method
vc	0.370	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.09	J/mol×K	363.35	Joback Method
cpg	172.44	J/mol×K	395.71	Joback Method
cpg	181.33	J/mol×K	428.07	Joback Method
cpg	189.77	J/mol×K	460.43	Joback Method
cpg	197.78	J/mol×K	492.80	Joback Method
cpg	205.37	J/mol×K	525.16	Joback Method
cpg	212.57	J/mol×K	557.52	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=R510924&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R510924&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>

# 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

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