

# 2-Hexanone, 1-chloro

Inchi:	InChI=1S/C6H11ClO/c1-2-3-4-6(8)5-7/h2-5H2,1H3
InchiKey:	FVXNLWRKEVZHKO-UHFFFAOYSA-N
Formula:	C6H11ClO
SMILES:	CCCCC(=O)CCl
Mol. weight [g/mol]:	134.60

## Physical Properties

Property code	Value	Unit	Source
gf	-141.21	kJ/mol	Joback Method
hf	-295.49	kJ/mol	Joback Method
hfus	17.09	kJ/mol	Joback Method
hvap	40.08	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.985		Crippen Method
mvol	109.210	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	943.00		NIST Webbook
rinpol	943.00		NIST Webbook
tb	427.98	K	Joback Method
tc	612.92	K	Joback Method
tf	237.23	K	Joback Method
vc	0.426	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.17	J/mol×K	427.98	Joback Method
cpg	248.12	J/mol×K	582.10	Joback Method
cpg	239.93	J/mol×K	551.27	Joback Method
cpg	231.35	J/mol×K	520.45	Joback Method
cpg	222.37	J/mol×K	489.63	Joback Method
cpg	212.98	J/mol×K	458.80	Joback Method
cpg	255.93	J/mol×K	612.92	Joback Method
dvisc	0.0003500	Paxs	427.98	Joback Method

dvisc	0.0004460	Paxs	396.19	Joback Method
dvisc	0.0005929	Paxs	364.40	Joback Method
dvisc	0.0008322	Paxs	332.61	Joback Method
dvisc	0.0012550	Paxs	300.81	Joback Method
dvisc	0.0020856	Paxs	269.02	Joback Method
dvisc	0.0039715	Paxs	237.23	Joback Method

## 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=R629746&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R629746&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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