

# E-2-(1-Chloro-ethylidene)-hexanal

<b>Inchi:</b>	InChI=1S/C8H13ClO/c1-3-4-5-8(6-10)7(2)9/h6H,3-5H2,1-2H3/b8-7-
<b>InchiKey:</b>	DOLCAJWTDNODFI-FPLPWBNLSA-N
<b>Formula:</b>	C8H13ClO
<b>SMILES:</b>	CCCCC(C=O)=C(C)Cl
<b>Mol. weight [g/mol]:</b>	160.64

## Physical Properties

Property code	Value	Unit	Source
gf	-31.85	kJ/mol	Joback Method
hf	-212.13	kJ/mol	Joback Method
hfus	20.54	kJ/mol	Joback Method
hvap	44.62	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.888		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1031.50		NIST Webbook
rinpol	1031.50		NIST Webbook
ripol	1446.20		NIST Webbook
tb	472.45	K	Joback Method
tc	664.80	K	Joback Method
tf	218.84	K	Joback Method
vc	0.531	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.15	J/mol×K	472.45	Joback Method
cpg	279.86	J/mol×K	504.51	Joback Method
cpg	290.95	J/mol×K	536.57	Joback Method
cpg	301.46	J/mol×K	568.63	Joback Method
cpg	311.41	J/mol×K	600.69	Joback Method
cpg	320.83	J/mol×K	632.74	Joback Method
cpg	329.76	J/mol×K	664.80	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=R153883&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R153883&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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	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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