

# 1,1,2-Trichlorocyclohexane

<b>Inchi:</b>	InChI=1S/C6H9Cl3/c7-5-3-1-2-4-6(5,8)9/h5H,1-4H2
<b>InchiKey:</b>	DAIRXERGRJFMSC-UHFFFAOYSA-N
<b>Formula:</b>	C6H9Cl3
<b>SMILES:</b>	C1C1CCCC1(Cl)Cl
<b>Mol. weight [g/mol]:</b>	187.50

## Physical Properties

Property code	Value	Unit	Source
gf	-24.90	kJ/mol	Joback Method
hf	-165.17	kJ/mol	Joback Method
hfus	10.49	kJ/mol	Joback Method
hvap	41.07	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.342		Crippen Method
mcvol	121.260	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	1191.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1191.00		NIST Webbook
tb	464.09	K	Joback Method
tc	702.00	K	Joback Method
tf	274.18	K	Joback Method
vc	0.449	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.11	J/molxK	464.09	Joback Method
cpg	233.87	J/molxK	503.74	Joback Method
cpg	246.48	J/molxK	543.39	Joback Method
cpg	258.06	J/molxK	583.04	Joback Method
cpg	268.76	J/molxK	622.70	Joback Method

cpg	278.72	J/mol×K	662.35	Joback Method
cpg	288.06	J/mol×K	702.00	Joback Method

## Sources

<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=R591463&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R591463&amp;Units=SI</a>
<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>

## 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>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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