

# 1,1,3,3-Tetrachlorocyclohexane

Inchi:	InChI=1S/C6H8Cl4/c7-5(8)2-1-3-6(9,10)4-5/h1-4H2
InchiKey:	PDMPQTTFFAJVGPNUHFFFAOYSA-N
Formula:	C6H8Cl4
SMILES:	C1C(Cl)CCCC(Cl)(Cl)C1
Mol. weight [g/mol]:	221.94

## Physical Properties

Property code	Value	Unit	Source
gf	-42.32	kJ/mol	Joback Method
hf	-165.67	kJ/mol	Joback Method
hfus	8.39	kJ/mol	Joback Method
hvap	44.31	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.908		Crippen Method
mcvol	133.500	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	1213.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1216.00		NIST Webbook
tb	501.76	K	Joback Method
tc	756.73	K	Joback Method
tf	328.00	K	Joback Method
vc	0.495	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.55	J/molxK	501.76	Joback Method
cpg	257.89	J/molxK	544.25	Joback Method
cpg	268.89	J/molxK	586.75	Joback Method
cpg	278.84	J/molxK	629.24	Joback Method

cpg	288.05	J/mol×K	671.74	Joback Method
cpg	296.84	J/mol×K	714.23	Joback Method
cpg	305.52	J/mol×K	756.73	Joback Method

## Sources

<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=R591478&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R591478&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>

## 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>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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