

# 5-chlorohexyl trichloroacetate

<b>Other names:</b>	1-Hexanol, 5-chloro, trichloroacetate
<b>Inchi:</b>	InChI=1S/C8H12Cl4O2/c1-6(9)4-2-3-5-14-7(13)8(10,11)12/h6H,2-5H2,1H3
<b>InchiKey:</b>	OVXVJMGTCAPECQ-UHFFFAOYSA-N
<b>Formula:</b>	C8H12Cl4O2
<b>SMILES:</b>	CC(Cl)CCCCOC(=O)C(Cl)(Cl)Cl
<b>Mol. weight [g/mol]:</b>	281.99

## Physical Properties

Property code	Value	Unit	Source
gf	-264.76	kJ/mol	Joback Method
hf	-530.24	kJ/mol	Joback Method
hfus	25.11	kJ/mol	Joback Method
hvap	58.41	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.697		Crippen Method
mcvol	179.980	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1518.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1585.00		NIST Webbook
ripol	2186.00		NIST Webbook
ripol	2205.00		NIST Webbook
ripol	2164.00		NIST Webbook
tb	604.78	K	Joback Method
tc	814.70	K	Joback Method
tf	359.18	K	Joback Method
vc	0.686	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.10	J/mol×K	604.78	Joback Method

cpg	398.94	J/molxK	639.77	Joback Method
cpg	409.06	J/molxK	674.75	Joback Method
cpg	418.49	J/molxK	709.74	Joback Method
cpg	427.28	J/molxK	744.73	Joback Method
cpg	435.44	J/molxK	779.72	Joback Method
cpg	443.01	J/molxK	814.70	Joback Method
dvisc	0.0027302	Paxs	359.18	Joback Method
dvisc	0.0013799	Paxs	400.11	Joback Method
dvisc	0.0007916	Paxs	441.05	Joback Method
dvisc	0.0004991	Paxs	481.98	Joback Method
dvisc	0.0003382	Paxs	522.91	Joback Method
dvisc	0.0002425	Paxs	563.85	Joback Method
dvisc	0.0001819	Paxs	604.78	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R112020&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R112020&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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