

# 6-chloroheptyl dichloroacetate

<b>Other names:</b>	1-Heptanol, 6-chloro, dichloroacetate
<b>Inchi:</b>	InChI=1S/C9H15Cl3O2/c1-7(10)5-3-2-4-6-14-9(13)8(11)12/h7-8H,2-6H2,1H3
<b>InchiKey:</b>	VJXZLHXTUIKGPD-UHFFFAOYSA-N
<b>Formula:</b>	C9H15Cl3O2
<b>SMILES:</b>	CC(Cl)CCCCCOC(=O)C(Cl)Cl
<b>Mol. weight [g/mol]:</b>	261.57

## Physical Properties

Property code	Value	Unit	Source
gf	-249.69	kJ/mol	Joback Method
hf	-531.67	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.521		Crippen Method
mcvol	181.830	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1604.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1582.00		NIST Webbook
ripol	2289.00		NIST Webbook
ripol	2317.00		NIST Webbook
ripol	2306.00		NIST Webbook
ripol	2289.00		NIST Webbook
tb	593.02	K	Joback Method
tc	788.71	K	Joback Method
tf	323.11	K	Joback Method
vc	0.699	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.32	J/mol×K	593.02	Joback Method

cpg	419.47	J/molxK	625.64	Joback Method
cpg	431.00	J/molxK	658.25	Joback Method
cpg	441.90	J/molxK	690.87	Joback Method
cpg	452.21	J/molxK	723.48	Joback Method
cpg	461.92	J/molxK	756.10	Joback Method
cpg	471.06	J/molxK	788.71	Joback Method
dvisc	0.0036788	Paxs	323.11	Joback Method
dvisc	0.0016526	Paxs	368.10	Joback Method
dvisc	0.0008837	Paxs	413.08	Joback Method
dvisc	0.0005344	Paxs	458.06	Joback Method
dvisc	0.0003536	Paxs	503.05	Joback Method
dvisc	0.0002504	Paxs	548.03	Joback Method
dvisc	0.0001868	Paxs	593.02	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=R111814&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R111814&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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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