

# 5-chlorooctyl dichloroacetate

<b>Other names:</b>	1-Octanol, 5-chloro, dichloroacetate
<b>Inchi:</b>	InChI=1S/C10H17Cl3O2/c1-2-5-8(11)6-3-4-7-15-10(14)9(12)13/h8-9H,2-7H2,1H3
<b>InchiKey:</b>	WCLXKRAF5OJBAM-UHFFFAOYSA-N
<b>Formula:</b>	C10H17Cl3O2
<b>SMILES:</b>	CCCC(CI)CCCCOC(=O)C(CI)CI
<b>Mol. weight [g/mol]:</b>	275.60

## Physical Properties

Property code	Value	Unit	Source
gf	-241.27	kJ/mol	Joback Method
hf	-552.31	kJ/mol	Joback Method
hfus	29.99	kJ/mol	Joback Method
hvap	59.39	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.911		Crippen Method
mcvol	195.920	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1667.00		NIST Webbook
ripol	2343.00		NIST Webbook
ripol	2361.00		NIST Webbook
ripol	2371.00		NIST Webbook
ripol	2343.00		NIST Webbook
tb	615.90	K	Joback Method
tc	809.16	K	Joback Method
tf	334.38	K	Joback Method
vc	0.754	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	455.66	J/molxK	615.90	Joback Method
cpg	468.53	J/molxK	648.11	Joback Method
cpg	480.73	J/molxK	680.32	Joback Method
cpg	492.28	J/molxK	712.53	Joback Method
cpg	503.19	J/molxK	744.74	Joback Method
cpg	513.48	J/molxK	776.95	Joback Method
cpg	523.15	J/molxK	809.16	Joback Method
dvisc	0.0033761	Paxs	334.38	Joback Method
dvisc	0.0014970	Paxs	381.30	Joback Method
dvisc	0.0007933	Paxs	428.22	Joback Method
dvisc	0.0004765	Paxs	475.14	Joback Method
dvisc	0.0003137	Paxs	522.06	Joback Method
dvisc	0.0002213	Paxs	568.98	Joback Method
dvisc	0.0001646	Paxs	615.90	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R112213&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R112213&amp;Units=SI</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

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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