

# 2-chlorooctyl trichloroacetate

<b>Other names:</b>	1-Octanol, 2-chloro, trichloroacetate
<b>Inchi:</b>	InChI=1S/C10H16Cl4O2/c1-2-3-4-5-6-8(11)7-16-9(15)10(12,13)14/h8H,2-7H2,1H3
<b>InchiKey:</b>	RIWGCMWHKHEPNH-UHFFFAOYSA-N
<b>Formula:</b>	C10H16Cl4O2
<b>SMILES:</b>	CCCCCCC(Cl)COC(=O)C(Cl)(Cl)Cl
<b>Mol. weight [g/mol]:</b>	310.05

## Physical Properties

Property code	Value	Unit	Source
gf	-247.92	kJ/mol	Joback Method
hf	-571.52	kJ/mol	Joback Method
hfus	30.29	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.478		Crippen Method
mcvol	208.160	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1670.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1670.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2218.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2176.00		NIST Webbook
tb	650.54	K	Joback Method
tc	854.25	K	Joback Method
tf	381.72	K	Joback Method
vc	0.798	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	484.42	J/molxK	650.54	Joback Method
cpg	496.64	J/molxK	684.49	Joback Method
cpg	508.09	J/molxK	718.44	Joback Method
cpg	518.80	J/molxK	752.39	Joback Method
cpg	528.80	J/molxK	786.35	Joback Method
cpg	538.14	J/molxK	820.30	Joback Method
cpg	546.84	J/molxK	854.25	Joback Method
dvisc	0.0022272	Paxs	381.72	Joback Method
dvisc	0.0010938	Paxs	426.52	Joback Method
dvisc	0.0006150	Paxs	471.33	Joback Method
dvisc	0.0003821	Paxs	516.13	Joback Method
dvisc	0.0002562	Paxs	560.93	Joback Method
dvisc	0.0001822	Paxs	605.74	Joback Method
dvisc	0.0001358	Paxs	650.54	Joback Method

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R112139&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## 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>mccvol:</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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