

# Octyl dichloroacetate

<b>Other names:</b>	1-Octanol, dichloroacetate
<b>Inchi:</b>	InChI=1S/C10H18Cl2O2/c1-2-3-4-5-6-7-8-14-10(13)9(11)12/h9H,2-8H2,1H3
<b>InchiKey:</b>	HBWBXXRQGCPRB-UHFFFAOYSA-N
<b>Formula:</b>	C10H18Cl2O2
<b>SMILES:</b>	CCCCCCCCOC(=O)C(Cl)Cl
<b>Mol. weight [g/mol]:</b>	241.16
<b>CAS:</b>	83004-98-2

## Physical Properties

Property code	Value	Unit	Source
gf	-226.90	kJ/mol	Joback Method
hf	-531.29	kJ/mol	Joback Method
hfus	29.31	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.694		Crippen Method
mcvol	183.680	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1484.30		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1481.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1950.00		NIST Webbook
tb	578.91	K	Joback Method
tc	764.42	K	Joback Method
tf	319.46	K	Joback Method
vc	0.712	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.73	J/molxK	578.91	Joback Method
cpg	441.05	J/molxK	609.83	Joback Method
cpg	453.75	J/molxK	640.75	Joback Method
cpg	465.85	J/molxK	671.67	Joback Method
cpg	477.36	J/molxK	702.58	Joback Method
cpg	488.28	J/molxK	733.50	Joback Method
cpg	498.63	J/molxK	764.42	Joback Method
dvisc	0.0032066	Paxs	319.46	Joback Method
dvisc	0.0015197	Paxs	362.70	Joback Method
dvisc	0.0008444	Paxs	405.94	Joback Method
dvisc	0.0005254	Paxs	449.19	Joback Method
dvisc	0.0003553	Paxs	492.43	Joback Method
dvisc	0.0002560	Paxs	535.67	Joback Method
dvisc	0.0001937	Paxs	578.91	Joback Method

## Sources

<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=C83004982&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C83004982&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>

## 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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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