

# Oxirane, (trichloromethyl)-

<b>Other names:</b>	Propane, 1,1,1-trichloro-2,3-epoxy- Trichloropropene oxide 1,1,1-Trichloro-2-propene oxide 1,1,1-Trichloro-2,3-epoxypropane 1,1,1-Trichloropropane 2,3-epoxide 1,1,1-Trichloropropene oxide 1,1,1-Trichloropropene 2,3-oxide 1,1,1-Trichloropropylene oxide 1,2-Epoxy-3,3,3-trichloropropane 3,3,3-Trichloro-1,2-epoxypropane 3,3,3-Trichloroepoxypropane 3,3,3-Trichloropropene oxide 3,3,3-Trichloropropylene oxide 1,1,1-Trichloropropene-2,3-epoxide Propane, 1,2-epoxy-3,3,3-trichloro- TCPO 1,1,1-Trichloropropane-2,3-oxide Trichloromethyloxirane 2-Trichloromethyloxirane NSC 136558 3,3,3-Trichloro-2-epoxypropane
<b>Inchi:</b>	InChI=1S/C3H3Cl3O/c4-3(5,6)2-1-7-2/h2H,1H2
<b>InchiKey:</b>	VFEXYZINKMLLAK-UHFFFAOYSA-N
<b>Formula:</b>	C3H3Cl3O
<b>SMILES:</b>	C1C(Cl)(Cl)C1O1
<b>Mol. weight [g/mol]:</b>	161.41
<b>CAS:</b>	3083-23-6

## Physical Properties

Property code	Value	Unit	Source
gf	-83.94	kJ/mol	Joback Method
hf	-220.42	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	38.55	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.755		Crippen Method

mvol	84.860	ml/mol	McGowan Method
pc	4583.94	kPa	Joback Method
rinpol	885.00		NIST Webbook
tb	410.79	K	Joback Method
tc	635.10	K	Joback Method
tf	260.26	K	Joback Method
vc	0.318	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.07	J/molxK	410.79	Joback Method
cpg	145.71	J/molxK	448.17	Joback Method
cpg	152.53	J/molxK	485.56	Joback Method
cpg	158.61	J/molxK	522.94	Joback Method
cpg	164.01	J/molxK	560.33	Joback Method
cpg	168.80	J/molxK	597.71	Joback Method
cpg	173.04	J/molxK	635.10	Joback Method
dvisc	0.0033927	Paxs	260.26	Joback Method
dvisc	0.0023728	Paxs	285.35	Joback Method
dvisc	0.0017582	Paxs	310.44	Joback Method
dvisc	0.0013625	Paxs	335.52	Joback Method
dvisc	0.0010940	Paxs	360.61	Joback Method
dvisc	0.0009039	Paxs	385.70	Joback Method
dvisc	0.0007644	Paxs	410.79	Joback Method

## Sources

**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)

**McGowan Method:**

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

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3083236&Units=SI>

## 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>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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