Oxirane, (trichloromethyl)-

Other names:	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
Inchi:	InChI=1S/C3H3Cl3O/c4-3(5,6)2-1-7-2/h2H,1H2
InchiKey:	VFEXYZINKMLLAK-UHFFFAOYSA-N
Formula:	C3H3Cl3O
SMILES:	ClC(Cl)(Cl)C1CO1
Mol. weight [g/mol]:	161.41
CAS:	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

mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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