

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:	C1C(Cl)(Cl)C1O1
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

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 ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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