Clorethate

Other names:	Bis(2,2,2-trichloroethyl) carbonate
	Ethanol, 2,2,2-trichloro-, carbonate (2:1)
	Carbonic acid, bis(2,2,2-trichloroethyl) ester
	Cloretat
	Cloretate
	SKF 12866
	2,2,2-Trichloroethyl carbonate
	Chlorethate
	SK&F 12866
	Bis-(2,2,2-trichlorethyl)ester kyseliny uhlicite
	NSC 15887
Inchi:	InChI=1S/C5H4Cl6O3/c6-4(7,8)1-13-3(12)14-2-5(9,10)11/h1-2H2
InchiKey:	IEPBPSSCIZTJIF-UHFFFAOYSA-N
Formula:	C5H4Cl6O3
SMILES:	O=C(OCC(Cl)(Cl)Cl)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	324.80
CAS:	5634-37-7

Physical Properties

Property code	Value	Unit	Source
gf	-413.60	kJ/mol	Joback Method
hf	-635.49	kJ/mol	Joback Method
hfus	23.04	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.880		Crippen Method
mcvol	168.060	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	630.63	K	Joback Method
tc	865.33	K	Joback Method
tf	424.86	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.73	J/mol×K	630.63	Joback Method
cpg	324.10	J/mol×K	669.75	Joback Method
cpg	329.80	J/mol×K	708.86	Joback Method
cpg	334.88	J/mol×K	747.98	Joback Method
cpg	339.39	J/mol×K	787.10	Joback Method
cpg	343.37	J/mol×K	826.21	Joback Method
cpg	346.87	J/mol×K	865.33	Joback Method
dvisc	0.0012760	Pa×s	424.86	Joback Method
dvisc	0.0007826	Pa×s	459.16	Joback Method
dvisc	0.0005138	Pa×s	493.45	Joback Method
dvisc	0.0003562	Pa×s	527.75	Joback Method
dvisc	0.0002583	Pa×s	562.04	Joback Method
dvisc	0.0001943	Pa×s	596.34	Joback Method
dvisc	0.0001508	Pa×s	630.63	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5634377&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume