Acetaldehyde, bis(2-chloroethyl) acetal

Other names:	Di(2-chloroethyl)acetal
	Ethane, 1,1'-(ethylidene)bis(oxy)bis(2-chloro-
	1,1-Bis(2-chloroethoxy)ethane
	1,1'-(Ethylidene)bis(oxy)bis(2-chloroethane)
	2,2-Di-(2'-chloroethoxy)-ethane
	Ethane,-1,1-di(2-chloroehtoxy)
	bis(2-chloroethyl)acetaldehyde acetal
Inchi:	InChI=1S/C6H12Cl2O2/c1-6(9-4-2-7)10-5-3-8/h6H,2-5H2,1H3
InchiKey:	KHNOWHUSVXGGLG-UHFFFAOYSA-N
Formula:	C6H12Cl2O2
SMILES:	CC(OCCCl)OCCCl
Mol. weight [g/mol]:	187.06
CAS:	14689-97-5

Physical Properties

Property code	Value	Unit	Source
gf	-236.66	kJ/mol	Joback Method
hf	-468.37	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	42.15	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.843		Crippen Method
mcvol	131.620	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
tb	455.94	K	Joback Method
tc	639.24	K	Joback Method
tf	246.68	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.76	J/mol×K	639.24	Joback Method
cpg	256.50	J/mol×K	455.94	Joback Method

cpg	266.52	J/mol×K	486.49	Joback Method
cpg	276.23	J/mol×K	517.04	Joback Method
cpg	285.62	J/mol×K	547.59	Joback Method
cpg	294.67	J/mol×K	578.14	Joback Method
cpg	303.39	J/mol×K	608.69	Joback Method
dvisc	0.0002230	Pa×s	455.94	Joback Method
dvisc	0.0036333	Pa×s	246.68	Joback Method
dvisc	0.0017107	Pa×s	281.56	Joback Method
dvisc	0.0009509	Pa×s	316.43	Joback Method
dvisc	0.0005940	Pa×s	351.31	Joback Method
dvisc	0.0004039	Pa×s	386.19	Joback Method
dvisc	0.0002928	Pa×s	421.06	Joback Method
hvapt	59.40	kJ/mol	407.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14689975&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
hvapt: Enthalpy of vaporization at a given temperature
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