2-Chloroethyl (2-chloroethoxy)ethyl sulfide

Inchi: InChI=1S/C6H12Cl2OS/c7-1-3-9-4-6-10-5-2-8/h1-6H2
InchiKey: YTSIBAYOCLBBIG-UHFFFAOYSA-N
Formula: C6H12Cl2OS
SMILES: ClCCOCCSCCCl
Mol. weight [g/mol]: 203.13

Physical Properties

Property code	Value	Unit	Source
gf	-96.10	kJ/mol	Joback Method
hf	-289.00	kJ/mol	Joback Method
hfus	25.01	kJ/mol	Joback Method
hvap	46.95	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	2.214		Crippen Method
mcvol	142.100	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1472.60		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1472.60		NIST Webbook
rinpol	1418.00		NIST Webbook
tb	502.74	K	Joback Method
tc	703.34	K	Joback Method
tf	273.85	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.92	J/mol×K	502.74	Joback Method
cpg	290.47	J/mol×K	536.17	Joback Method
cpg	300.57	J/mol×K	569.61	Joback Method
cpg	310.23	J/mol×K	603.04	Joback Method

cpg	319.44	J/mol×K	636.47	Joback Method
cpg	328.21	J/mol×K	669.91	Joback Method
cpg	336.52	J/mol×K	703.34	Joback Method

Sources

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=R41388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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