2-Chloroethyl vinyl sulfide

Other names: Ethene, [(2-chloroethyl)thio]-
Inchi: InChI=1S/C4H7ClS/c1-2-6-4-3-5/h2H,1,3-4H2
InchiKey: KCCNHHACDJEDCX-UHFFFAOYSA-N
Formula: C4H7ClS
SMILES: C=CSCCCl
Mol. weight [g/mol]: 122.62
CAS: 81142-02-1

Physical Properties

Property code	Value	Unit	Source
gf	91.83	kJ/mol	Joback Method
hf	25.67	kJ/mol	Joback Method
hfus	13.16	kJ/mol	Joback Method
hvap	35.03	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	2.102		Crippen Method
mcvol	91.510	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
rinpol	903.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	874.00		NIST Webbook
tb	393.81	K	Joback Method
tc	598.20	K	Joback Method
tf	197.40	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	144.10	J/mol×K	393.81	Joback Method
cpg	151.63	J/mol×K	427.88	Joback Method
cpg	158.81	J/mol×K	461.94	Joback Method
cpg	165.64	J/mol×K	496.01	Joback Method
cpg	172.14	J/mol×K	530.07	Joback Method
cpg	178.31	J/mol×K	564.14	Joback Method
cpg	184.17	J/mol×K	598.20	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=C81142021&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