(2-Chloroethylthio)ethyl vinyl sulfide

Inchi: InChI=1S/C6H11ClS2/c1-2-8-5-6-9-4-3-7/h2H,1,3-6H2
InchiKey: CBVAXGNCAZECCK-UHFFFAOYSA-N
Formula: C6H11ClS2
SMILES: C=CSCCSCCCl
Mol. weight [g/mol]: 182.74

Physical Properties

Property code	Value	Unit	Source
gf	141.79	kJ/mol	Joback Method
hf	26.26	kJ/mol	Joback Method
hfus	22.47	kJ/mol	Joback Method
hvap	46.30	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.835		Crippen Method
mcvol	136.040	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1413.40		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1413.40		NIST Webbook
tb	508.35	K	Joback Method
tc	730.99	K	Joback Method
tf	254.34	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.33	J/mol×K	508.35	Joback Method
cpg	272.30	J/mol×K	545.46	Joback Method
cpg	282.69	J/mol×K	582.56	Joback Method
cpg	292.49	J/mol×K	619.67	Joback Method
cpg	301.73	J/mol×K	656.78	Joback Method

cpg	310.40	J/mol×K	693.89	Joback Method
cpg	318.52	J/mol×K	730.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41495&Units=SI

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