2-Chlorovinyl 2-hydroxyethyl sulfide

Inchi: InChI=1S/C4H7ClOS/c5-1-3-7-4-2-6/h1,3,6H,2,4H2/b3-1+
InchiKey: YXIDSJSRQIFGOB-HNQUOIGGSA-N
Formula: C4H7ClOS
SMILES: OCCSC=CCl
Mol. weight [g/mol]: 138.62

Physical Properties

Property code	Value	Unit	Source
gf	-52.61	kJ/mol	Joback Method
hf	-134.77	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	52.34	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.422		Crippen Method
mcvol	97.380	ml/mol	McGowan Method
pc	4577.74	kPa	Joback Method
rinpol	1114.00		NIST Webbook
rinpol	1114.00		NIST Webbook
tb	493.47	K	Joback Method
tc	692.24	K	Joback Method
tf	254.90	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.31	J/mol×K	493.47	Joback Method
cpg	185.06	J/mol×K	526.60	Joback Method
cpg	191.43	J/mol×K	559.73	Joback Method
cpg	197.44	J/mol×K	592.85	Joback Method
cpg	203.12	J/mol×K	625.98	Joback Method
cpg	208.47	J/mol×K	659.11	Joback Method
cpg	213.51	J/mol×K	692.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502324&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
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