(2-Chloroethylthiopropyl)-(2-chloroethylthioethyl) sulfide

Inchi: InChI=1S/C9H18Cl2S3/c1-9(14-5-3-11)8-13-7-6-12-4-2-10/h9H,2-8H2,1H3
InchiKey: XMISXRLGQMFZPP-UHFFFAOYSA-N
Formula: C9H18Cl2S3
SMILES: CC(CSCCSCCCl)SCCCl
Mol. weight [g/mol]: 293.34

Physical Properties

Property code	Value	Unit	Source
gf	97.96	kJ/mol	Joback Method
hf	-140.24	kJ/mol	Joback Method
hfus	36.33	kJ/mol	Joback Method
hvap	64.46	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	4.052		Crippen Method
mcvol	211.200	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	2252.00		NIST Webbook
rinpol	2252.00		NIST Webbook
tb	686.08	K	Joback Method
tc	917.66	K	Joback Method
tf	339.23	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.34	J/mol×K	686.08	Joback Method
cpg	509.16	J/mol×K	724.68	Joback Method
cpg	522.02	J/mol×K	763.27	Joback Method
cpg	533.93	J/mol×K	801.87	Joback Method
cpg	544.90	J/mol×K	840.47	Joback Method
cpg	554.94	J/mol×K	879.07	Joback Method
cpg	564.06	J/mol×K	917.66	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=R422996&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