2-Chloroethyl 3-chloropropyl disulfide

Inchi: InChI=1S/C5H10Cl2S2/c6-2-1-4-8-9-5-3-7/h1-5H2
InchiKey: HKWIQEYFFLRIDR-UHFFFAOYSA-N
Formula: C5H10Cl2S2
SMILES: ClCCCSSCCCl
Mol. weight [g/mol]: 205.17

Physical Properties

Property code	Value	Unit	Source
gf	33.60	kJ/mol	Joback Method
hf	-94.27	kJ/mol	Joback Method
hfus	25.36	kJ/mol	Joback Method
hvap	49.13	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	3.236		Crippen Method
mcvol	138.490	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1427.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1427.00		NIST Webbook
tb	526.22	K	Joback Method
tc	752.80	K	Joback Method
tf	274.75	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.39	J/mol×K	526.22	Joback Method
cpg	270.34	J/mol×K	563.98	Joback Method
cpg	279.76	J/mol×K	601.75	Joback Method
cpg	288.64	J/mol×K	639.51	Joback Method
cpg	296.98	J/mol×K	677.27	Joback Method
cpg	304.79	J/mol×K	715.03	Joback Method
cpg	312.08	J/mol×K	752.80	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=R422976&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