1-(2-Chloroethyldithio)-4-(2-chloroethylthio)butan

Other names: 1-(2-Chloroethylthio)-4-(2-chloroethyldithio)butane
Inchi: InChI=1S/C8H16Cl2S3/c9-3-7-11-5-1-2-6-12-13-8-4-10/h1-8H2
InchiKey: HKUHXMSHILQITM-UHFFFAOYSA-N
Formula: C8H16Cl2S3
SMILES: ClCCSCCCCSSCCCl
Mol. weight [g/mol]: 279.31

Physical Properties

Property code	Value	Unit	Source
gf	91.98	kJ/mol	Joback Method
hf	-114.32	kJ/mol	Joback Method
hfus	37.26	kJ/mol	Joback Method
hvap	62.62	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.359		Crippen Method
mcvol	197.110	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	663.64	K	Joback Method
tc	895.12	K	Joback Method
tf	342.96	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.51	J/mol×K	663.64	Joback Method
cpg	457.42	J/mol×K	702.22	Joback Method
cpg	469.46	J/mol×K	740.80	Joback Method
cpg	480.64	J/mol×K	779.38	Joback Method
cpg	490.96	J/mol×K	817.96	Joback Method
cpg	500.44	J/mol×K	856.54	Joback Method

cpg	509.08	J/mol×K	895.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R499659&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

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