Bis[(2-chloroethyltyio)ethyl] sulfide

Other names: bis-[(2-Chloroethylthio)ethyl] sulfide
Inchi: InChI=1S/C8H16Cl2S3/c9-1-3-11-5-7-13-8-6-12-4-2-10/h1-8H2
InchiKey: MINLWGQAHTUHFI-UHFFFAOYSA-N
Formula: C8H16Cl2S3
SMILES: ClCCSCCSCCSCCCl
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	-3.13		Crippen Method
logp	3.664		Crippen Method
mcvol	197.110	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
rinpol	2222.00		NIST Webbook
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook
rinpol	2141.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360307&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