1,4-Bis(2-chloroethylthio)butane

Inchi: InChI=1S/C8H16Cl2S2/c9-3-7-11-5-1-2-6-12-8-4-10/h1-8H2
InchiKey: AYSIRJGVBLMLAS-UHFFFAOYSA-N
Formula: C8H16Cl2S2
SMILES: ClCCSCCCCSCCCl
Mol. weight [g/mol]: 247.25
CAS: 142868-93-7

Physical Properties

Property code	Value	Unit	Source
gf	58.86	kJ/mol	Joback Method
hf	-156.19	kJ/mol	Joback Method
hfus	33.13	kJ/mol	Joback Method
hvap	55.81	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.711		Crippen Method
mcvol	180.760	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1759.00		NIST Webbook
tb	594.86	K	Joback Method
tc	809.64	K	Joback Method
tf	308.56	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.65	J/mol×K	594.86	Joback Method
cpg	407.66	J/mol×K	630.66	Joback Method
cpg	419.94	J/mol×K	666.45	Joback Method
cpg	431.50	J/mol×K	702.25	Joback Method
cpg	442.36	J/mol×K	738.04	Joback Method
cpg	452.54	J/mol×K	773.84	Joback Method
cpg	462.04	J/mol×K	809.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142868937&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