1,3-Bis(2-chloroethylthio)propane

Inchi: InChI=1S/C7H14Cl2S2/c8-2-6-10-4-1-5-11-7-3-9/h1-7H2
InchiKey: YHRGRBPJIRKFND-UHFFFAOYSA-N
Formula: C7H14Cl2S2
SMILES: ClCCSCCCSCCCl
Mol. weight [g/mol]: 233.22
CAS: 63905-10-2

Physical Properties

Property code	Value	Unit	Source
gf	50.44	kJ/mol	Joback Method
hf	-135.55	kJ/mol	Joback Method
hfus	30.54	kJ/mol	Joback Method
hvap	53.58	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	3.321		Crippen Method
mcvol	166.670	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1811.00		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1811.00		NIST Webbook
tb	571.98	K	Joback Method
tc	790.53	K	Joback Method
tf	297.29	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.10	J/mol×K	571.98	Joback Method
cpg	360.23	J/mol×K	608.41	Joback Method
cpg	371.69	J/mol×K	644.83	Joback Method
cpg	382.48	J/mol×K	681.26	Joback Method
cpg	392.62	J/mol×K	717.68	Joback Method
cpg	402.12	J/mol×K	754.11	Joback Method

cpg	410.98	J/mol×K	790.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63905102&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