Sulfide, bis(2-chloropropyl)

Other names:	Bis(2-chloropropyl)sulfide
	(-)-«alpha»,«alpha»'-Dimethyl-«beta»,«beta»'-bischloroethyl sulfide
	Propane, 1,1'-thiobis(2-chloro-
	TL 293
	Propane, 2-chloro-3-(2-chloropropylthio)-
Inchi:	InChI=1S/C6H12Cl2S/c1-5(7)3-9-4-6(2)8/h5-6H,3-4H2,1-2H3
InchiKey:	AQHTWLYIOSPNMG-UHFFFAOYSA-N
Formula:	C6H12Cl2S
SMILES:	CC(Cl)CSCC(C)Cl
Mol. weight [g/mol]:	187.13
CAS:	22535-54-2

Physical Properties

Property code	Value	Unit	Source
gf	4.02	kJ/mol	Joback Method
hf	-167.34	kJ/mol	Joback Method
hfus	16.77	kJ/mol	Joback Method
hvap	43.76	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.974		Crippen Method
mcvol	136.230	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	479.44	K	Joback Method
tc	691.09	K	Joback Method
tf	221.62	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.36	J/mol×K	479.44	Joback Method
cpg	269.74	J/mol×K	514.71	Joback Method
cpg	280.54	J/mol×K	549.99	Joback Method
cpg	290.78	J/mol×K	585.26	Joback Method

cpg	300.46	J/mol×K	620.54	Joback Method
cpg	309.60	J/mol×K	655.81	Joback Method
cpg	318.21	J/mol×K	691.09	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=C22535542&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume