2-Chloroethyl 5-chloropentyl sulfide

Inchi: InChI=1S/C7H14Cl2S/c8-4-2-1-3-6-10-7-5-9/h1-7H2
InchiKey: MEQTYPQVPQPQQT-UHFFFAOYSA-N
Formula: C7H14Cl2S
SMILES: ClCCCCCSCCCl
Mol. weight [g/mol]: 201.16

Physical Properties

Property code	Value	Unit	Source
gf	17.32	kJ/mol	Joback Method
hf	-177.42	kJ/mol	Joback Method
hfus	26.41	kJ/mol	Joback Method
hvap	46.76	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	3.368		Crippen Method
mcvol	150.320	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1274.00		NIST Webbook
tb	503.20	K	Joback Method
tc	702.67	K	Joback Method
tf	262.89	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.88	J/mol×K	503.20	Joback Method
cpg	311.71	J/mol×K	536.44	Joback Method
cpg	322.97	J/mol×K	569.69	Joback Method
cpg	333.67	J/mol×K	602.93	Joback Method
cpg	343.83	J/mol×K	636.18	Joback Method
cpg	353.46	J/mol×K	669.42	Joback Method
cpg	362.59	J/mol×K	702.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502295&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