2-Chloroethyl-2-chloropropyl sulfide

Inchi: InChI=1S/C5H10Cl2S/c1-5(7)4-8-3-2-6/h5H,2-4H2,1H3
InchiKey: UXBWKLYRAKLSAF-UHFFFAOYSA-N
Formula: C5H10Cl2S
SMILES: CC(Cl)CSCCCl
Mol. weight [g/mol]: 173.10

Physical Properties

Property code	Value	Unit	Source
gf	-1.96	kJ/mol	Joback Method
hf	-141.42	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	41.92	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.586		Crippen Method
mcvol	122.140	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	1223.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1214.00		NIST Webbook
tb	457.00	K	Joback Method
tc	666.69	K	Joback Method
tf	225.35	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.23	J/mol×K	457.00	Joback Method
cpg	227.99	J/mol×K	491.95	Joback Method
cpg	237.28	J/mol×K	526.90	Joback Method
cpg	246.10	J/mol×K	561.85	Joback Method
cpg	254.46	J/mol×K	596.80	Joback Method
cpg	262.37	J/mol×K	631.74	Joback Method
cpg	269.84	J/mol×K	666.69	Joback Method

Sources

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=R422921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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