(2-Chloroethylthioethyl) (2-chloroethylthiopropyl) ether

Inchi: InChI=1S/C9H18Cl2OS2/c1-9(14-6-3-11)8-12-4-7-13-5-2-10/h9H,2-8H2,1H3

InchiKey: SSFZHVATVUJHDL-UHFFFAOYSA-N

Formula: C9H18Cl2OS2

SMILES: CC(COCCSCCCl)SCCCl

Mol. weight [g/mol]: 277.27

Physical Properties

Property code	Value	Unit	Source
gf	-40.16	kJ/mol	Joback Method
hf	-314.33	kJ/mol	Joback Method
hfus	33.38	kJ/mol	Joback Method
hvap	60.05	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	3.336		Crippen Method
mcvol	200.720	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	639.72	K	Joback Method
tc	852.74	K	Joback Method
tf	327.06	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.37	J/mol×K	639.72	Joback Method
cpg	482.20	J/mol×K	675.22	Joback Method
cpg	495.25	J/mol×K	710.73	Joback Method
cpg	507.51	J/mol×K	746.23	Joback Method
cpg	518.99	J/mol×K	781.74	Joback Method
cpg	529.69	J/mol×K	817.24	Joback Method
cpg	539.60	J/mol×K	852.74	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=R502304&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