(3-Chloropropylthioethyl1)-(2-chloroethylthioethy ether

Other names: (3-Chloropropylthioethyl)-(2-chloroethylthioethyl) ether
Inchi: InChI=1S/C9H18Cl2OS2/c10-2-1-6-13-8-4-12-5-9-14-7-3-11/h1-9H2
InchiKey: YOBXSBPCGUGRDK-UHFFFAOYSA-N
Formula: C9H18Cl2OS2
SMILES: ClCCCSCCOCCSCCCl
Mol. weight [g/mol]: 277.27

Physical Properties

Property code	Value	Unit	Source
gf	-37.72	kJ/mol	Joback Method
hf	-309.05	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	60.44	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	3.337		Crippen Method
mcvol	200.720	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
tb	640.16	K	Joback Method
tc	849.12	K	Joback Method
tf	342.06	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.88	J/mol×K	640.16	Joback Method
cpg	481.41	J/mol×K	674.99	Joback Method
cpg	494.19	J/mol×K	709.81	Joback Method
cpg	506.23	J/mol×K	744.64	Joback Method
cpg	517.53	J/mol×K	779.47	Joback Method
cpg	528.08	J/mol×K	814.30	Joback Method
cpg	537.90	J/mol×K	849.12	Joback Method

Sources

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=U360306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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