Bis[(3-chloropropylthio)ethyl] ether

Inchi: InChI=1S/C10H20Cl2OS2/c11-3-1-7-14-9-5-13-6-10-15-8-2-4-12/h1-10H2
InchiKey: SNJWALBVDPAWLN-UHFFFAOYSA-N
Formula: C10H20Cl2OS2
SMILES: ClCCCSCCOCCSCCCCl
Mol. weight [g/mol]: 291.30

Physical Properties

Property code	Value	Unit	Source
gf	-29.30	kJ/mol	Joback Method
hf	-329.69	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.727		Crippen Method
mcvol	214.810	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2022.00		NIST Webbook
rinpol	2022.00		NIST Webbook
tb	663.04	K	Joback Method
tc	868.96	K	Joback Method
tf	353.33	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.48	J/mol×K	663.04	Joback Method
cpg	532.63	J/mol×K	697.36	Joback Method
cpg	545.98	J/mol×K	731.68	Joback Method
cpg	558.54	J/mol×K	766.00	Joback Method
cpg	570.32	J/mol×K	800.32	Joback Method
cpg	581.31	J/mol×K	834.64	Joback Method
cpg	591.53	J/mol×K	868.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R423028&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