Ethane, 1-chloro-2-[(2-ethoxyethyl)thio]-

Other names: (2-Chloroethylthio)ethyl ethyl ether
Inchi: InChI=1S/C6H13ClOS/c1-2-8-4-6-9-5-3-7/h2-6H2,1H3
InchiKey: UXYAOPOYEMOOHI-UHFFFAOYSA-N
Formula: C6H13ClOS
SMILES: CCOCCSCCCl
Mol. weight [g/mol]: 168.69
CAS: 114811-33-5

Physical Properties

Property code	Value	Unit	Source
gf	-84.17	kJ/mol	Joback Method
hf	-273.26	kJ/mol	Joback Method
hfus	20.81	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.995		Crippen Method
mcvol	129.860	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1169.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1169.00		NIST Webbook
tb	465.31	K	Joback Method
tc	660.22	K	Joback Method
tf	243.93	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.05	J/mol×K	465.31	Joback Method
cpg	266.00	J/mol×K	497.79	Joback Method
cpg	276.55	J/mol×K	530.28	Joback Method
cpg	286.69	J/mol×K	562.76	Joback Method

cpg	296.42	J/mol×K	595.25	Joback Method
cpg	305.74	J/mol×K	627.73	Joback Method
cpg	314.65	J/mol×K	660.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C114811335&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

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