2-Chloroethyl ethyl sulfide

Other names:	Ethane, 1-chloro-2-(ethylthio)-
	«beta»-Ethylmerkaptoethylchlorid
	Ethyl 2-chloroethyl sulfide
	Sulfide, chloroethyl ethyl
	Sulfide, 2-chloroethyl ethyl
	1-Chloro-2-(ethylthio)ethane
	2-(Ethylthio)chloroethane
	2-Chloroethyl ethyl thioether
	2-Ethylthioethyl chloride
	Chlordiethylsulfid
	Ethyl «beta»-chloroethyl sulfide
	Half-mustard gas
	h-MG
	NSC 10977
	Half-sulfur mustard
	2-chloroethyl ethyl sulphide
Inchi:	InChI=1S/C4H9ClS/c1-2-6-4-3-5/h2-4H2,1H3
InchiKey:	GBNVXYXIRHSYEG-UHFFFAOYSA-N
Formula:	C4H9ClS
SMILES:	CCSCCCl
Mol. weight [g/mol]:	124.63
CAS:	693-07-2

Physical Properties

Property code	Value	Unit	Source
gf	3.99	kJ/mol	Joback Method
hf	-99.76	kJ/mol	Joback Method
hfus	14.44	kJ/mol	Joback Method
hvap	35.70	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.978		Crippen Method
mcvol	95.810	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	430.20	K	NIST Webbook
tc	596.96	K	Joback Method
tf	199.16	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.31	J/mol×K	397.13	Joback Method
cpg	166.65	J/mol×K	430.44	Joback Method
cpg	174.64	J/mol×K	463.74	Joback Method
cpg	182.31	J/mol×K	497.05	Joback Method
cpg	189.65	J/mol×K	530.35	Joback Method
cpg	196.66	J/mol×K	563.66	Joback Method
cpg	203.36	J/mol×K	596.96	Joback Method
hvapt	44.40	kJ/mol	313.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.20	K	6.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C693072&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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume