Bis(«beta»-chloroethyl) sulfoxide

Other names:	1,1'-Sulfinylbis[2-chloroethane]
	1-chloro-2-(2-chloroethylsulfinyl)ethane
	Bis(2-chloroethyl) sulfoxide
	Ethane, 1,1'-sulfinylbis[2-chloro-
	H Sulfoxide
	Mustard gas sulfoxide
	Mustard sulfone
	NSC 141393
	Sulfoxide, bis(2-chloroethyl)
	Yperite sulfoxide
Inchi:	InChI=1S/C4H8Cl2OS/c5-1-3-8(7)4-2-6/h1-4H2
InchiKey:	NOMHBBFEJSVGSC-UHFFFAOYSA-N
Formula:	C4H8Cl2OS
SMILES:	O=S(CCCl)CCCl
Mol. weight [g/mol]:	175.08
CAS:	5819-08-9

Physical Properties

Property code	Value	Unit	Source
gf	-258.77	kJ/mol	Joback Method
hf	-363.11	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
log10ws	-1.16		Aqueous Solubility Prediction Method
logp	1.213		Crippen Method
mcvol	113.920	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	424.06	K	Joback Method
tc	616.88	K	Joback Method
tf	231.16	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.92	J/mol×K	424.06	Joback Method
cpg	202.17	J/mol×K	456.20	Joback Method
cpg	210.07	J/mol×K	488.33	Joback Method
cpg	217.62	J/mol×K	520.47	Joback Method
cpg	224.82	J/mol×K	552.61	Joback Method
cpg	231.68	J/mol×K	584.75	Joback Method
cpg	238.20	J/mol×K	616.88	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5819089&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume