Ethane, 1,1'-sulfinylbis[2-chloro-

Other names:	1,1'-Sulfinylbis[2-chloroethane]
	1-chloro-2-(2-chloroethylsulfinyl)ethane
	Bis(2-chloroethyl) sulfoxide
	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

Physical Properties

Property code	Value	Unit	Source
hf	-259.60	kJ/mol	Cheméo Relay (1.0)
hfus	22.26	kJ/mol	Joback Method
hvap	85.11	kJ/mol	Cheméo Relay (1.0)
ie	9.43	eV	Cheméo Relay (1.0)
log10ws	-1.16		Aqueous Solubility Prediction Method
logp	1.213		Crippen Method
mcvol	113.920	ml/mol	McGowan Method
rinpol	1365.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1367.00		NIST Webbook
tb	540.03	K	Cheméo Relay (1.0)
tf	370.36	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5819089&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point