1-Chloro-2-(2-chloroethanesulfonyl)ethane

Other names:	1-chloro-2-(2-chloroethylsulfonyl)ethane
	Bis(«beta»-chloroethyl) sulfone
	Ethane, 1,1'-sulfonylbis(2-chloro-
	H Sulfone
	Mustard gas sulfone
	Mustard sulfone
	NSC 26284
	Sulfone, bis(2-chloroethyl)
	Yperite sulfone
Inchi:	InChI=1S/C4H8Cl2O2S/c5-1-3-9(7,8)4-2-6/h1-4H2
InchiKey:	LUYAMNYBNTVQJG-UHFFFAOYSA-N
Formula:	C4H8Cl2O2S
SMILES:	O=S(=O)(CCCl)CCCl
Mol. weight [g/mol]:	191.08

Physical Properties

Property code	Value	Unit	Source
hf	-463.37	kJ/mol	Cheméo Relay (1.0)
hfus	25.89	kJ/mol	Joback Method
hvap	93.46	kJ/mol	Cheméo Relay (1.0)
log10ws	-1.50		Aqueous Solubility Prediction Method
logp	0.879		Crippen Method
mcvol	119.790	ml/mol	McGowan Method
tb	565.56	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.99	J/mol×K	413.56	Joback Method
cpg	215.40	J/mol×K	443.45	Joback Method
cpg	223.48	J/mol×K	473.34	Joback Method
cpg	231.24	J/mol×K	503.24	Joback Method
cpg	238.68	J/mol×K	533.13	Joback Method

cpg	245.79	J/mol×K	563.02	Joback Method
cpg	252.57	J/mol×K	592.91	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C471034&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature