O-Mustard

Other names:	Bis(2-chloroethylthioethyl) ether
	Ethane, 1,1'-oxybis(2-((2-chloroethyl)thio)-
	Ether, bis(2-(2-chloroethylmercapto)ethyl)
	Ether, bis(2-chloroethylthioethyl)
	Bis(«beta»-chloroethylthioethyl) ether
	2-2'-Di(3-chloroethylthio)-diethyl ether
	Dimustard ether
	bis-[(2-Chloroethylthio)ethy] ether
	Agent T
	NSC 58818
	O-Mustard T
Inchi:	InChI=1S/C8H16Cl2OS2/c9-1-5-12-7-3-11-4-8-13-6-2-10/h1-8H2
InchiKey:	FWVCSXWHVOOTFJ-UHFFFAOYSA-N
Formula:	C8H16Cl2OS2
SMILES:	ClCCSCCOCCSCCCl
Mol. weight [g/mol]:	263.25
CAS:	63918-89-8

Physical Properties

Property code	Value	Unit	Source
gf	-46.14	kJ/mol	Joback Method
hf	-288.41	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	58.22	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.947		Crippen Method
mcvol	186.630	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1982.60		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1982.60		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1987.80		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1979.60		NIST Webbook

rinpol	1974.00		NIST Webbook
ripol	3040.00		NIST Webbook
ripol	3040.30		NIST Webbook
tb	617.28	K	Joback Method
tc	829.60	K	Joback Method
tf	330.79	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.78	J/mol×K	617.28	Joback Method
cpg	431.59	J/mol×K	652.67	Joback Method
cpg	443.71	J/mol×K	688.05	Joback Method
cpg	455.14	J/mol×K	723.44	Joback Method
cpg	465.87	J/mol×K	758.83	Joback Method
cpg	475.90	J/mol×K	794.21	Joback Method
cpg	485.23	J/mol×K	829.60	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C63918898&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume