ETHANE, 1,1'-OXYBIS[2-(2-CHLOROETHYL)THIO-

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

Physical Properties

Property code	Value	Unit	Source
hfus	34.32	kJ/mol	Joback Method
hvap	83.64	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.75		Cheméo Relay (1.0)
logp	2.947		Crippen Method
mcvol	186.630	ml/mol	McGowan Method
rinpol	1974.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1987.80		NIST Webbook
rinpol	1982.60		NIST Webbook
rinpol	1982.60		NIST Webbook
rinpol	1979.60		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
ripol	3040.00		NIST Webbook
ripol	3040.30		NIST Webbook
tb	584.81	K	Cheméo Relay (1.0)

tf	252.46	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63918898&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point