Sesquimustard

Other names:	1,2-Bis(2-chloroethylthio)ethane
	Ethane, 1,2-bis(2-chloro-ethylthio)-
	Ethane, 1,2-bis((2-chloroethyl)mercapto)-
	HSM 1
	Sesqui-mustard Q
	Sesquisulfur Mustard
	SM 1
	SSM
	TL 86
	Bis(2-chloroethylthio)ethane
	1,2-Bis(«beta»-chloroethylthio)ethane
	1,8-Dichloro-3,6-dithiaoctane
	3,6-Dithia-1,8-octanedichloride
	Agent Q
	NSC 30025
Inchi:	InChI=1S/C6H12Cl2S2/c7-1-3-9-5-6-10-4-2-8/h1-6H2
InchiKey:	AMGNHZVUZWILSB-UHFFFAOYSA-N
Formula:	C6H12Cl2S2
SMILES:	ClCCSCCSCCCl
Mol. weight [g/mol]:	219.19
CAS:	3563-36-8

Physical Properties

Property code	Value	Unit	Source
gf	42.02	kJ/mol	Joback Method
hf	-114.91	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	51.35	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.930		Crippen Method
mcvol	152.580	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1703.30		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1688.80		NIST Webbook
rinpol	1684.00		NIST Webbook
tb	549.10	K	Joback Method

tc	771.60	K	Joback Method
tf	286.02	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.31	J/mol×K	549.10	Joback Method
cpg	314.43	J/mol×K	586.18	Joback Method
cpg	324.93	J/mol×K	623.27	Joback Method
cpg	334.84	J/mol×K	660.35	Joback Method
cpg	344.14	J/mol×K	697.44	Joback Method
cpg	352.85	J/mol×K	734.52	Joback Method
cpg	360.98	J/mol×K	771.60	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3563368&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume