Mustard Gas

Other names:

1,1'-Thiobis(2-chloroethane)
1-Chloro-2-(«beta»-chloroethylthio)ethane
1-Chloro-2-(Â«betaÂ»-chloroethylthio)ethane
1-chloro-2-(.beta.-chloroethylthio)ethane
2,2'-Dichlorodiethyl sulfide
2,2'-Dichloroethyl sulfide
Agent THD
Agent hd
Bis(2-chloroethyl) sulfide
Bis(2-chloroethyl) sulphide
Bis(«beta»-chloroethyl) sulfide
Bis(Â«betaÂ»-chloroethyl) sulfide
Di(2-chloroethyl) sulfide
Distilled mustard
Ethane, 1,1'-thiobis[2-chloro-
Gelbkreuz
HD
Iprit
Kampfstoff "lost"
Kampstoff lost
Lost
Mustard
Mustard HD
Mustard Vapor
Mustard, sulfur
S Lost
S Mustard
S-Yperite
Schwefel-lost
Senfgas
Sulfide, bis(2-chloroethyl)
Sulfur mustard
Sulfur mustard gas
THD
Yellow cross gas
Yellow cross liquid
Yperite
beta,beta'-Dichlorodiethyl sulfide
bis(.beta.-chloroethyl) sulfide
«beta»,«beta»'-Dichloroethyl sulfide

	«beta»,«beta»-Dichloroethyl sulfide
	«beta»-Chloroethylisobutyl sulfide
	Â«betaÂ»,Â«betaÂ»'-Dichloroethyl sulfide
	Â«betaÂ»,Â«betaÂ»-Dichloroethyl sulfide
	Â«betaÂ»-Chloroethylisobutyl sulfide
Inchi:	InChI=1S/C4H8Cl2S/c5-1-3-7-4-2-6/h1-4H2
InchiKey:	QKSKPIVNLNLAAV-UHFFFAOYSA-N
Formula:	C4H8Cl2S
SMILES:	ClCCSCCCl
Mol. weight [g/mol]:	159.08
CAS:	505-60-2

Physical Properties

Property code	Value	Unit	Source
chl	-3163.50 ± 1.30	kJ/mol	NIST Webbook
gf	-7.94	kJ/mol	Joback Method
hf	-115.50	kJ/mol	Joback Method
hfl	-200.50 ± 1.60	kJ/mol	NIST Webbook
hfus	18.64	kJ/mol	Joback Method
hvap	59.80 ± 2.10	kJ/mol	NIST Webbook
log10ws	-1.69		Crippen Method
logp	2.197		Crippen Method
mcvol	108.050	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1123.80		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1177.07		NIST Webbook
rinpol	1177.07		NIST Webbook
rinpol	1173.25		NIST Webbook
rinpol	1173.59		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1175.50		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1172.70		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1124.80		NIST Webbook
rinpol	1172.70		NIST Webbook
rinpol	1174.10		NIST Webbook
rinpol	1178.00		NIST Webbook

rinpol	1183.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1123.80		NIST Webbook
rinpol	1173.59		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1820.00		NIST Webbook
tb	489.20	K	NIST Webbook
tc	641.96	K	Joback Method
tf	229.08	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.38	J/mol×K	538.26	Joback Method
cpg	196.08	J/mol×K	503.69	Joback Method
cpg	188.42	J/mol×K	469.13	Joback Method
cpg	223.12	J/mol×K	641.96	Joback Method
cpg	216.89	J/mol×K	607.39	Joback Method
cpg	210.31	J/mol×K	572.82	Joback Method
cpg	180.38	J/mol×K	434.56	Joback Method
hsubt	77.20	kJ/mol	275.00	NIST Webbook
hsubt	80.90	kJ/mol	270.50	NIST Webbook
hvapt	50.30	kJ/mol	373.00	NIST Webbook
hvapt	59.60	kJ/mol	323.00	NIST Webbook
psub	3.34e-03	kPa	283.15	Vapor Pressure of Solid Bis(2-chloroethyl) Sulfide
psub	1.86e-03	kPa	278.15	Vapor Pressure of Solid Bis(2-chloroethyl) Sulfide
psub	9.84e-04	kPa	273.15	Vapor Pressure of Solid Bis(2-chloroethyl) Sulfide

psub	4.90e-04	kPa	268.15	Vapor Pressure of Solid Bis(2-chloroethyl) Sulfide
psub	2.41e-04	kPa	263.15	Vapor Pressure of Solid Bis(2-chloroethyl) Sulfide
psub	1.18e-04	kPa	258.15	Vapor Pressure of Solid Bis(2-chloroethyl) Sulfide
psub	5.60e-05	kPa	253.15	Vapor Pressure of Solid Bis(2-chloroethyl) Sulfide
psub	2.77e-05	kPa	248.15	Vapor Pressure of Solid Bis(2-chloroethyl) Sulfide
psub	4.81e-03	kPa	286.15	Vapor Pressure of Solid Bis(2-chloroethyl) Sulfide

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.80721e+01
Coeff. B	-6.30480e+03
Coeff. C	-2.05220e+01
Temperature range (K), min.	375.03
Temperature range (K), max.	514.61

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1867.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C505602&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Vapor Pressure of Solid Bis(2-chloroethyl) Sulfide: https://www.doi.org/10.1021/je060077o

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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor 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