

Disulfide, bis(2-chloroethyl)

Other names:	1,6-Dichloro-3,4-dithiahexane 2,2'-Dichloroethyl disulfide Bis(2-chloroethyl) disulfide Mustard disulfide
Inchi:	InChI=1S/C4H8Cl2S2/c5-1-3-7-8-4-2-6/h1-4H2
InchiKey:	XDFZUXHZXUFQOS-UHFFFAOYSA-N
Formula:	C4H8Cl2S2
SMILES:	CICCCSSCCI
Mol. weight [g/mol]:	191.14
CAS:	1002-41-1

Physical Properties

Property code	Value	Unit	Source
gf	25.18	kJ/mol	Joback Method
hf	-73.63	kJ/mol	Joback Method
hfus	22.77	kJ/mol	Joback Method
hvap	46.90	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.845		Crippen Method
mcvol	124.400	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
rinpol	1391.20		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1391.00		NIST Webbook
tb	503.34	K	Joback Method
tc	734.06	K	Joback Method
tf	263.48	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.45	J/molxK	503.34	Joback Method
cpg	228.07	J/molxK	541.79	Joback Method

cpg	236.24	J/mol×K	580.25	Joback Method
cpg	243.95	J/mol×K	618.70	Joback Method
cpg	251.20	J/mol×K	657.16	Joback Method
cpg	257.98	J/mol×K	695.61	Joback Method
cpg	264.31	J/mol×K	734.06	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1002411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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