2-CHLORO-2'-HYDROXYDIETHYL SULFIDE

Other names:	Half mustard gas
	Half sulfur mustard
	Hemisulfur mustard
	HSM
	Mustard chlorohydrin
	Sulfide, 2-chloroethyl 2-hydroxyethyl
	Sulfur half-mustard
	2-Chloroethyl 2-hydroxyethyl sulfide
	2-Chloroethyl-2'-hydroxyethyl sulfide
	2-Hydroxyethyl 2-chloroethyl sulfide
	«beta»-Chloroethyl «beta»-hydroxyethyl sulfide
	2-((2-Chloroethyl)thio)ethanol
	2-Chloro-2'-hydroxydiethylsulfide
	NSC 30024
Inchi:	InChI=1S/C4H9ClOS/c5-1-3-7-4-2-6/h6H,1-4H2
InchiKey:	ZGFPMAMREQRRRB-UHFFFAOYSA-N
Formula:	C4H9ClOS
SMILES:	OCCSCCCl
Mol. weight [g/mol]:	140.64

Physical Properties

Property code	Value	Unit	Source
hfus	18.53	kJ/mol	Joback Method
hvap	71.46	kJ/mol	Cheméo Relay (1.0)
ie	9.51	eV	Cheméo Relay (1.0)
logp	0.951		Crippen Method
mcvol	101.680	ml/mol	McGowan Method
rinpol	1132.00		NIST Webbook
rinpol	1177.50		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1177.50		NIST Webbook
rinpol	1132.00		NIST Webbook
tb	510.86	K	Cheméo Relay (1.0)
tf	232.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.35	J/mol×K	489.31	Joback Method
cpg	203.74	J/mol×K	520.95	Joback Method
cpg	210.81	J/mol×K	552.60	Joback Method
cpg	217.56	J/mol×K	584.24	Joback Method
cpg	224.00	J/mol×K	615.88	Joback Method
cpg	230.13	J/mol×K	647.52	Joback Method
cpg	235.96	J/mol×K	679.17	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C693301&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

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point