(Chloromethyl)thiirane

Other names:	Chloropropylene sulfide
	Epithiochlorohydrin
	Propane, 1-chloro-2,3-epithio-
	Thiirane, (chloromethyl)-
	Thiirane, 2-(chloromethyl)-
	Thioepichlorhydrin
	Thioepichlorohydrin
	1-Chloro-2,3-epithiopropane
	2-(Chloromethyl)ethylene sulfide
	2-(Chloromethyl)thiirane
	2-Thiiranylmethyl chloride
	3-Chloropropylene sulfide
	Chloropropylene sulphide
	3-Chloropropene sulfide
	3-Chloro-1,2-propylene sulfide
Inchi:	InChI=1S/C3H5ClS/c4-1-3-2-5-3/h3H,1-2H2
InchiKey:	XRWMHJJHPQTTLQ-UHFFFAOYSA-N
Formula:	C3H5ClS
SMILES:	ClCC1CS1
Mol. weight [g/mol]:	108.59
CAS:	3221-15-6

Physical Properties

Property code	Value	Unit	Source
gf	63.06	kJ/mol	Joback Method
hf	-2.93	kJ/mol	Joback Method
hfus	9.51	kJ/mol	Joback Method
hvap	32.38	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.341		Crippen Method
mcvol	70.860	ml/mol	McGowan Method
pc	4966.33	kPa	Joback Method
rinpol	835.00		NIST Webbook
tb	360.04	K	Joback Method
tc	568.99	K	Joback Method
tf	254.88	K	Joback Method
vc	0.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	105.50	J/mol×K	360.04	Joback Method
cpg	113.18	J/mol×K	394.87	Joback Method
cpg	120.30	J/mol×K	429.69	Joback Method
cpg	126.89	J/mol×K	464.52	Joback Method
cpg	133.00	J/mol×K	499.34	Joback Method
cpg	138.65	J/mol×K	534.17	Joback Method
cpg	143.89	J/mol×K	568.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3221156&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