Thiirane, 2-(1-chloroethyl)

Inchi: InChI=1S/C4H7ClS/c1-3(5)4-2-6-4/h3-4H,2H2,1H3
InchiKey: WOIHFPJCIFTANY-UHFFFAOYSA-N
Formula: C4H7ClS
SMILES: CC(Cl)C1CS1
Mol. weight [g/mol]: 122.62

Physical Properties

Property code	Value	Unit	Source
gf	69.04	kJ/mol	Joback Method
hf	-28.85	kJ/mol	Joback Method
hfus	8.58	kJ/mol	Joback Method
hvap	34.22	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.729		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
rinpol	858.00		NIST Webbook
tb	382.48	K	Joback Method
tc	595.22	K	Joback Method
tf	251.15	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.74	J/mol×K	382.48	Joback Method
cpg	148.32	J/mol×K	417.94	Joback Method
cpg	157.23	J/mol×K	453.39	Joback Method
cpg	165.52	J/mol×K	488.85	Joback Method
cpg	173.23	J/mol×K	524.31	Joback Method
cpg	180.39	J/mol×K	559.77	Joback Method
cpg	187.06	J/mol×K	595.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R512282&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