Thiirane, 2-methyl-2-chloromethyl

Inchi: InChI=1S/C4H7ClS/c1-4(2-5)3-6-4/h2-3H2,1H3
InchiKey: RYVLXOUOFMZVRE-UHFFFAOYSA-N
Formula: C4H7ClS
SMILES: CC1(CCl)CS1
Mol. weight [g/mol]: 122.62

Physical Properties

Property code	Value	Unit	Source
gf	65.99	kJ/mol	Joback Method
hf	-8.33	kJ/mol	Joback Method
hfus	5.81	kJ/mol	Joback Method
hvap	33.46	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.731		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
rinpol	861.00		NIST Webbook
tb	383.16	K	Joback Method
tc	600.60	K	Joback Method
tf	290.05	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.27	J/mol×K	383.16	Joback Method
cpg	149.24	J/mol×K	419.40	Joback Method
cpg	158.11	J/mol×K	455.64	Joback Method
cpg	166.01	J/mol×K	491.88	Joback Method
cpg	173.07	J/mol×K	528.12	Joback Method
cpg	179.42	J/mol×K	564.36	Joback Method
cpg	185.19	J/mol×K	600.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R512306&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