2,2-Dimethylthiirane

Other names: Thiirane, 2,2-dimethyl-
Inchi: InChI=1S/C4H8S/c1-4(2)3-5-4/h3H2,1-2H3
InchiKey: HGJOFJDIHKHKAU-UHFFFAOYSA-N
Formula: C4H8S
SMILES: CC1(C)CS1
Mol. weight [g/mol]: 88.17
CAS: 3772-13-2

Physical Properties

Property code	Value	Unit	Source
chl	-3295.00 ± 1.00	kJ/mol	NIST Webbook
gf	77.92	kJ/mol	Joback Method
hf	7.41	kJ/mol	Joback Method
hfl	-24.00 ± 1.00	kJ/mol	NIST Webbook
hfus	1.61	kJ/mol	Joback Method
hvap	29.07	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.512		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	4869.76	kPa	Joback Method
rinpol	728.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	692.00		NIST Webbook
tb	345.73	K	Joback Method
tc	553.36	K	Joback Method
tf	260.13	K	Joback Method
vc	0.261	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.52	J/mol×K	345.73	Joback Method
cpg	125.43	J/mol×K	380.33	Joback Method
cpg	135.24	J/mol×K	414.94	Joback Method

cpg	144.05	J/mol×K	449.54	Joback Method
cpg	151.98	J/mol×K	484.15	Joback Method
cpg	159.14	J/mol×K	518.75	Joback Method
cpg	165.64	J/mol×K	553.36	Joback Method
hvapt	37.00	kJ/mol	373.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3772132&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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