1,3-Oxathiolane, 2,2-dimethyl-

Other names: 2,2-Dimethyl-1,3-oxathiolane
Inchi: InChI=1S/C5H10OS/c1-5(2)6-3-4-7-5/h3-4H2,1-2H3
InchiKey: XLSCZCCJPDTCGU-UHFFFAOYSA-N
Formula: C5H10OS
SMILES: CC1(C)OCCS1
Mol. weight [g/mol]: 118.20
CAS: 5684-31-1

Physical Properties

Property code	Value	Unit	Source
gf	-23.98	kJ/mol	Joback Method
hf	-157.55	kJ/mol	Joback Method
hfus	7.98	kJ/mol	Joback Method
hvap	36.15	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.486		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
rinpol	853.00		NIST Webbook
rinpol	853.00		NIST Webbook
tb	404.10	K	Joback Method
tc	629.69	K	Joback Method
tf	290.93	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.67	J/mol×K	404.10	Joback Method
cpg	185.79	J/mol×K	441.70	Joback Method
cpg	197.77	J/mol×K	479.30	Joback Method
cpg	208.73	J/mol×K	516.89	Joback Method
cpg	218.81	J/mol×K	554.49	Joback Method
cpg	228.12	J/mol×K	592.09	Joback Method

cpg	236.79	J/mol×K	629.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5684311&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

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