1,3-Oxathiane, 2,4,6-trimethyl-, (2«alpha»,4«alpha»,6«alpha»)-

Other names: 1,3-Oxathiane, 2,4,6-trimethyl-, cis,cis-
2,4,6-Trimethyl-1,3-oxathiane, (Z,Z)-
Inchi: InChI=1S/C7H14OS/c1-5-4-6(2)9-7(3)8-5/h5-7H,4H2,1-3H3/t5-,6+,7-/m1/s1
InchiKey: DUDZTWRICXYHEJ-DSYKOEDSSA-N
Formula: C7H14OS
SMILES: CC1CC(C)SC(C)O1
Mol. weight [g/mol]: 146.25
CAS: 22521-88-6

Physical Properties

Property code	Value	Unit	Source
gf	-29.17	kJ/mol	Joback Method
hf	-260.91	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	41.31	kJ/mol	Joback Method
ie	8.55	eV	NIST Webbook
log10ws	-2.45		Crippen Method
logp	2.263		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
tb	444.55	K	Joback Method
tc	662.56	K	Joback Method
tf	277.57	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.69	J/mol×K	444.55	Joback Method
cpg	268.35	J/mol×K	480.88	Joback Method
cpg	284.23	J/mol×K	517.22	Joback Method
cpg	299.33	J/mol×K	553.55	Joback Method
cpg	313.67	J/mol×K	589.89	Joback Method
cpg	327.26	J/mol×K	626.22	Joback Method

cpg	340.09	J/mol×K	662.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22521886&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume