

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

Other names:	1,3-Oxathiane, 2,4,6-trimethyl-, trans-2,4,cis-2,6- 2,4,6-Trimethyl-1,3-oxathiane, trans-2,4,cis-2,6-
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-FSDSQADBSA-N
Formula:	C7H14OS
SMILES:	CC1CC(C)SC(C)O1
Mol. weight [g/mol]:	146.25
CAS:	22425-90-7

## 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	8.58	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/molxK	444.55	Joback Method
cpg	268.35	J/molxK	480.88	Joback Method
cpg	284.23	J/molxK	517.22	Joback Method
cpg	299.33	J/molxK	553.55	Joback Method
cpg	313.67	J/molxK	589.89	Joback Method
cpg	327.26	J/molxK	626.22	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C22425907&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22425907&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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