

# 1,3-Oxathiolane, 2-ethyl-2,5-dimethyl-, trans-

<b>Inchi:</b>	InChI=1S/C7H14OS/c1-4-7(3)8-6(2)5-9-7/h6H,4-5H2,1-3H3/t6-,7+/m0/s1
<b>InchiKey:</b>	JMORGBZMPQAHJW-NKWVEPMBSA-N
<b>Formula:</b>	C7H14OS
<b>SMILES:</b>	CCC1(C)OC(C)CS1
<b>Mol. weight [g/mol]:</b>	146.25
<b>CAS:</b>	38384-69-9

## Physical Properties

Property code	Value	Unit	Source
gf	-14.85	kJ/mol	Joback Method
hf	-219.17	kJ/mol	Joback Method
hfus	14.23	kJ/mol	Joback Method
hvap	40.30	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.264		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
tb	445.19	K	Joback Method
tc	664.50	K	Joback Method
tf	309.23	K	Joback Method
vc	0.432	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.89	J/mol×K	445.19	Joback Method
cpg	268.52	J/mol×K	481.74	Joback Method
cpg	283.04	J/mol×K	518.29	Joback Method
cpg	296.56	J/mol×K	554.84	Joback Method
cpg	309.20	J/mol×K	591.40	Joback Method
cpg	321.06	J/mol×K	627.95	Joback Method
cpg	332.26	J/mol×K	664.50	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=C38384699&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38384699&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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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