

# trans-2-Isopropyl-5-methyl-1,3-oxathiolane

<b>Inchi:</b>	InChI=1S/C7H14OS/c1-5(2)7-8-6(3)4-9-7/h5-7H,4H2,1-3H3/t6-,7+/m0/s1
<b>InchiKey:</b>	ODRUEFNMTNWJNO-NKWVEPMBSA-N
<b>Formula:</b>	C7H14OS
<b>SMILES:</b>	CC1CSC(C(C)C)O1
<b>Mol. weight [g/mol]:</b>	146.25
<b>CAS:</b>	38384-67-7

## Physical Properties

Property code	Value	Unit	Source
gf	-11.80	kJ/mol	Joback Method
hf	-239.69	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	41.06	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.120		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	444.51	K	Joback Method
tc	659.36	K	Joback Method
tf	270.33	K	Joback Method
vc	0.428	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.16	J/molxK	444.51	Joback Method
cpg	267.93	J/molxK	480.32	Joback Method
cpg	282.89	J/molxK	516.13	Joback Method
cpg	297.06	J/molxK	551.94	Joback Method
cpg	310.46	J/molxK	587.75	Joback Method
cpg	323.11	J/molxK	623.56	Joback Method
cpg	335.04	J/molxK	659.36	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=C38384677&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38384677&amp;Units=SI</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>mccvol:</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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