

# 1,2-Oxathiolane, 4-methyl

Inchi:	InChI=1S/C4H8OS/c1-4-2-5-6-3-4/h4H,2-3H2,1H3
InchiKey:	CTCQRZKJIABGRB-UHFFFAOYSA-N
Formula:	C4H8OS
SMILES:	CC1COSC1
Mol. weight [g/mol]:	104.17

## Physical Properties

Property code	Value	Unit	Source
gf	-26.91	kJ/mol	Joback Method
hf	-152.15	kJ/mol	Joback Method
hfus	11.69	kJ/mol	Joback Method
hvap	35.08	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	1.301		Crippen Method
mvol	78.580	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
rinpol	981.00		NIST Webbook
rinpol	981.00		NIST Webbook
tb	380.98	K	Joback Method
tc	598.45	K	Joback Method
tf	255.76	K	Joback Method
vc	0.268	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.54	J/mol×K	380.98	Joback Method
cpg	146.53	J/mol×K	417.23	Joback Method
cpg	156.91	J/mol×K	453.47	Joback Method
cpg	166.70	J/mol×K	489.72	Joback Method
cpg	175.93	J/mol×K	525.96	Joback Method
cpg	184.62	J/mol×K	562.21	Joback Method
cpg	192.79	J/mol×K	598.45	Joback Method

# Sources

<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=R63099&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R63099&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>

# 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>rinpola:</b>	Non-polar retention indices
<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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