

# 2-Oxazolidinethione, 4,4-dimethyl-

<b>Other names:</b>	4,4-Dimethyloxazolidine-2-thione Oxazolidine-2-thione, 4,4-dimethyl- 4,4-Dimethyloxazoline-2-thiol 4,4-Dimethyl-2-oxazolidinethione
<b>Inchi:</b>	InChI=1S/C5H9NOS/c1-5(2)3-7-4(8)6-5/h3H2,1-2H3,(H,6,8)
<b>InchiKey:</b>	VIMMIOUDVZQBAK-UHFFFAOYSA-N
<b>Formula:</b>	C5H9NOS
<b>SMILES:</b>	CC1(C)COC(=S)N1
<b>Mol. weight [g/mol]:</b>	131.20
<b>CAS:</b>	54013-55-7

## Physical Properties

Property code	Value	Unit	Source
gf	114.72	kJ/mol	Joback Method
hf	-49.90	kJ/mol	Joback Method
hfus	19.95	kJ/mol	Joback Method
hvap	44.58	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	0.670		Crippen Method
mcvol	98.350	ml/mol	McGowan Method
pc	5153.45	kPa	Joback Method
tb	477.46	K	Joback Method
tc	719.23	K	Joback Method
tf	376.18	K	Joback Method
vc	0.350	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.67	J/molxK	477.46	Joback Method
cpg	210.63	J/molxK	517.76	Joback Method
cpg	220.61	J/molxK	558.05	Joback Method
cpg	229.77	J/molxK	598.35	Joback Method
cpg	238.26	J/molxK	638.64	Joback Method

cpg	246.24	J/mol×K	678.94	Joback Method
cpg	253.87	J/mol×K	719.23	Joback Method

## Sources

<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=C54013557&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54013557&amp;Units=SI</a>
<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>

## 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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