

# Thiolan-4-on-3-thiol, 2-methyl

<b>Other names:</b>	Thiolan-4-one, 2-methyl-3-mercapto 2-Methylthiolan-4-one-3-thiol
<b>Inchi:</b>	InChI=1S/C5H8OS2/c1-3-5(7)4(6)2-8-3/h3,5,7H,2H2,1H3
<b>InchiKey:</b>	XXRXAVULMYKULG-UHFFFAOYSA-N
<b>Formula:</b>	C5H8OS2
<b>SMILES:</b>	CC1SCC(=O)C1S
<b>Mol. weight [g/mol]:</b>	148.25

## Physical Properties

Property code	Value	Unit	Source
gf	-33.28	kJ/mol	Joback Method
hf	-160.35	kJ/mol	Joback Method
hfus	10.92	kJ/mol	Joback Method
hvap	43.47	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	0.989		Crippen Method
mcvol	104.720	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
rinpol	1237.00		NIST Webbook
rinpol	1239.00		NIST Webbook
tb	502.92	K	Joback Method
tc	766.27	K	Joback Method
tf	340.90	K	Joback Method
vc	0.362	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.36	J/molxK	502.92	Joback Method
cpg	225.62	J/molxK	546.81	Joback Method
cpg	238.18	J/molxK	590.70	Joback Method
cpg	250.02	J/molxK	634.59	Joback Method
cpg	261.12	J/molxK	678.48	Joback Method
cpg	271.46	J/molxK	722.37	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=R69809&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R69809&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>rinpol:</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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