

# 2-Methylthiolan-3-thiol

Inchi:	InChI=1S/C5H10S2/c1-4-5(6)2-3-7-4/h4-6H,2-3H2,1H3
InchiKey:	DPEXPKGKIRGPKJ-UHFFFAOYSA-N
Formula:	C5H10S2
SMILES:	CC1SCCC1S
Mol. weight [g/mol]:	134.26

## Physical Properties

Property code	Value	Unit	Source
gf	89.31	kJ/mol	Joback Method
hf	-22.65	kJ/mol	Joback Method
hfus	11.41	kJ/mol	Joback Method
hvap	39.22	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.810		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
rinpol	1042.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1042.00		NIST Webbook
tb	435.10	K	Joback Method
tc	678.52	K	Joback Method
tf	272.68	K	Joback Method
vc	0.355	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.46	J/molxK	435.10	Joback Method
cpg	204.37	J/molxK	475.67	Joback Method
cpg	217.43	J/molxK	516.24	Joback Method
cpg	229.68	J/molxK	556.81	Joback Method
cpg	241.15	J/molxK	597.38	Joback Method
cpg	251.87	J/molxK	637.95	Joback Method
cpg	261.86	J/molxK	678.52	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=R125774&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R125774&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>hvpap:</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>rlnpol:</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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