

# 2-methyl-5-thianonane

Inchi:	InChI=1S/C9H20S/c1-4-5-7-10-8-6-9(2)3/h9H,4-8H2,1-3H3
InchiKey:	PSEUPOGUWGH LIJ-UHFFFAOYSA-N
Formula:	C9H20S
SMILES:	CCCCSCCC(C)C
Mol. weight [g/mol]:	160.32

## Physical Properties

Property code	Value	Unit	Source
gf	55.58	kJ/mol	Joback Method
hf	-192.50	kJ/mol	Joback Method
hfus	19.67	kJ/mol	Joback Method
hvap	42.06	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.566		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
tb	473.66	K	Joback Method
tc	661.48	K	Joback Method
tf	210.59	K	Joback Method
vc	0.588	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.57	J/molxK	473.66	Joback Method
cpg	345.86	J/molxK	504.96	Joback Method
cpg	360.50	J/molxK	536.27	Joback Method
cpg	374.52	J/molxK	567.57	Joback Method
cpg	387.92	J/molxK	598.87	Joback Method
cpg	400.72	J/molxK	630.17	Joback Method

## Sources

<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=R156293&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R156293&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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