

# 1,2,4,6-Tetrathiepane, 3,5,7-trimethyl, #2

Inchi:	InChI=1S/C6H12S4/c1-4-7-5(2)9-10-6(3)8-4/h4-6H,1-3H3
InchiKey:	WMWRKEXBIGLGBW-UHFFFAOYSA-N
Formula:	C6H12S4
SMILES:	CC1SSC(C)SC(C)S1
Mol. weight [g/mol]:	212.42

## Physical Properties

Property code	Value	Unit	Source
gf	156.01	kJ/mol	Joback Method
hf	21.35	kJ/mol	Joback Method
hfus	17.80	kJ/mol	Joback Method
hvap	52.18	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.886		Crippen Method
mcvol	149.940	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	1535.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1526.00		NIST Webbook
tb	542.48	K	Joback Method
tc	821.95	K	Joback Method
tf	486.56	K	Joback Method
vc	0.478	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.07	J/molxK	542.48	Joback Method
cpg	332.22	J/molxK	589.06	Joback Method
cpg	348.20	J/molxK	635.64	Joback Method
cpg	363.03	J/molxK	682.22	Joback Method
cpg	376.73	J/molxK	728.79	Joback Method
cpg	389.29	J/molxK	775.37	Joback Method
cpg	400.73	J/molxK	821.95	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=R44615&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R44615&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>h vap:</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>r in pol:</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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