

# 1,2,3,5,6,8-hexathiacyclononane

<b>Inchi:</b>	InChI=1S/C3H6S6/c1-4-2-7-9-8-3-6-5-1/h1-3H2
<b>InchiKey:</b>	ZOJCTXCAPUGEKN-UHFFFAOYSA-N
<b>Formula:</b>	C3H6S6
<b>SMILES:</b>	C1SCSSSCSS1
<b>Mol. weight [g/mol]:</b>	234.47

## Physical Properties

Property code	Value	Unit	Source
gf	209.40	kJ/mol	Joback Method
hf	222.49	kJ/mol	Joback Method
hfus	9.93	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.017		Crippen Method
mcvol	140.370	ml/mol	McGowan Method
pc	6620.58	kPa	Joback Method
rinpol	1901.00		NIST Webbook
rinpol	1901.00		NIST Webbook
tb	592.05	K	Joback Method
tc	951.49	K	Joback Method
tf	625.33	K	Joback Method
vc	0.390	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.34	J/mol×K	592.05	Joback Method
cpg	268.22	J/mol×K	651.96	Joback Method
cpg	279.68	J/mol×K	711.86	Joback Method
cpg	289.74	J/mol×K	771.77	Joback Method
cpg	298.43	J/mol×K	831.67	Joback Method
cpg	305.79	J/mol×K	891.58	Joback Method
cpg	311.86	J/mol×K	951.49	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=R217006&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R217006&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>hvp:</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>rlnol:</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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