

# 2,4,4-trimethyl-3-thiahexane

Inchi:	InChI=1S/C8H18S/c1-6-8(4,5)9-7(2)3/h7H,6H2,1-5H3
InchiKey:	NCVWNQQEGJYSTR-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CCC(C)(C)SC(C)C
Mol. weight [g/mol]:	146.29

## Physical Properties

Property code	Value	Unit	Source
gf	50.00	kJ/mol	Joback Method
hf	-180.61	kJ/mol	Joback Method
hfus	9.67	kJ/mol	Joback Method
hvap	38.54	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.317		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpola	952.00		NIST Webbook
rinpola	952.00		NIST Webbook
rinpola	952.00		NIST Webbook
rinpola	952.00		NIST Webbook
tb	447.55	K	Joback Method
tc	649.97	K	Joback Method
tf	201.74	K	Joback Method
vc	0.520	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.43	J/molxK	447.55	Joback Method
cpg	305.13	J/molxK	481.29	Joback Method
cpg	320.01	J/molxK	515.02	Joback Method
cpg	334.09	J/molxK	548.76	Joback Method
cpg	347.41	J/molxK	582.50	Joback Method
cpg	359.99	J/molxK	616.23	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=R155572&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R155572&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>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>mcpvol:</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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