

# 3,5,6-trimethyl-4-thiaheptane

Inchi:	InChI=1S/C9H20S/c1-6-8(4)10-9(5)7(2)3/h7-9H,6H2,1-5H3
InchiKey:	VAMBGYNCDFSVMB-UHFFFAOYSA-N
Formula:	C9H20S
SMILES:	CCC(C)SC(C)C(C)C
Mol. weight [g/mol]:	160.32

## Physical Properties

Property code	Value	Unit	Source
gf	50.70	kJ/mol	Joback Method
hf	-203.06	kJ/mol	Joback Method
hfus	12.63	kJ/mol	Joback Method
hvap	41.28	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.563		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	1054.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1054.00		NIST Webbook
tb	472.78	K	Joback Method
tc	669.11	K	Joback Method
tf	180.59	K	Joback Method
vc	0.576	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.83	J/molxK	472.78	Joback Method
cpg	346.97	J/molxK	505.50	Joback Method
cpg	362.39	J/molxK	538.22	Joback Method
cpg	377.11	J/molxK	570.94	Joback Method
cpg	391.15	J/molxK	603.67	Joback Method

cpg	404.51	J/mol×K	636.39	Joback Method
cpg	417.22	J/mol×K	669.11	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=R156515&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R156515&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>hvac:</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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