

# 2,3-dimethyl-4-thiaheptane

Inchi:	InChI=1S/C8H18S/c1-5-6-9-8(4)7(2)3/h7-8H,5-6H2,1-4H3
InchiKey:	HMVSZFDLCPRNSL-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CCCSC(C)C(C)C
Mol. weight [g/mol]:	146.29

## Physical Properties

Property code	Value	Unit	Source
gf	44.72	kJ/mol	Joback Method
hf	-177.14	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	39.44	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	3.174		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
rinpol	1015.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1015.00		NIST Webbook
tb	450.34	K	Joback Method
tc	644.50	K	Joback Method
tf	184.32	K	Joback Method
vc	0.525	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.13	J/molxK	450.34	Joback Method
cpg	301.81	J/molxK	482.70	Joback Method
cpg	315.88	J/molxK	515.06	Joback Method
cpg	329.34	J/molxK	547.42	Joback Method
cpg	342.19	J/molxK	579.78	Joback Method
cpg	354.46	J/molxK	612.14	Joback Method
cpg	366.15	J/molxK	644.50	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>
<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=R155512&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R155512&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>

# 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>rinp:</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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