

# 2-methyl-3,4,5-trithiahexane

Inchi:	InChI=1S/C4H10S3/c1-4(2)6-7-5-3/h4H,1-3H3
InchiKey:	ZUJLLBXDHHTMEV-UHFFFAOYSA-N
Formula:	C4H10S3
SMILES:	CSSSC(C)C
Mol. weight [g/mol]:	154.32

## Physical Properties

Property code	Value	Unit	Source
gf	79.72	kJ/mol	Joback Method
hf	-5.56	kJ/mol	Joback Method
hfus	14.98	kJ/mol	Joback Method
hvap	44.56	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.054		Crippen Method
mcvol	116.270	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	1126.00		NIST Webbook
tb	496.82	K	Joback Method
tc	745.77	K	Joback Method
tf	223.04	K	Joback Method
vc	0.415	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.04	J/mol×K	496.82	Joback Method
cpg	227.67	J/mol×K	538.31	Joback Method
cpg	237.77	J/mol×K	579.80	Joback Method
cpg	247.33	J/mol×K	621.29	Joback Method
cpg	256.33	J/mol×K	662.79	Joback Method
cpg	264.74	J/mol×K	704.28	Joback Method
cpg	272.55	J/mol×K	745.77	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=R156035&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R156035&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>

# 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>mccvol:</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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