

# 1,2,4-Trithiolane, 3-methyl-5-pentyl

<b>Inchi:</b>	InChI=1S/C9H18S3/c1-3-4-5-6-9-7-10-12-8(2)11-9/h8-9H,3-7H2,1-2H3
<b>InchiKey:</b>	CKEAHKHPLAKFOJ-UHFFFAOYSA-N
<b>Formula:</b>	C9H18S3
<b>SMILES:</b>	CCCCC1CSSC(C)S1
<b>Mol. weight [g/mol]:</b>	222.43

## Physical Properties

Property code	Value	Unit	Source
gf	161.22	kJ/mol	Joback Method
hf	-59.33	kJ/mol	Joback Method
hfus	22.94	kJ/mol	Joback Method
hvap	53.18	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.409		Crippen Method
mvol	175.860	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	563.69	K	Joback Method
tc	802.80	K	Joback Method
tf	444.68	K	Joback Method
vc	0.610	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.49	J/mol×K	563.69	Joback Method
cpg	426.00	J/mol×K	603.54	Joback Method
cpg	443.38	J/mol×K	643.39	Joback Method
cpg	459.65	J/mol×K	683.24	Joback Method
cpg	474.85	J/mol×K	723.10	Joback Method
cpg	489.03	J/mol×K	762.95	Joback Method
cpg	502.23	J/mol×K	802.80	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=R54460&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R54460&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>h vap:</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>r in pol:</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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