

# 1,2,4-Trithiolane, 3-ethyl-5-(1-methylethyl), #2

Inchi:	InChI=1S/C7H14S3/c1-4-6-8-7(5(2)3)10-9-6/h5-7H,4H2,1-3H3
InchiKey:	DLGUSEQUYDDHKA-UHFFFAOYSA-N
Formula:	C7H14S3
SMILES:	CCC1SSC(C(C)C)S1
Mol. weight [g/mol]:	194.38

## Physical Properties

Property code	Value	Unit	Source
gf	154.04	kJ/mol	Joback Method
hf	-17.17	kJ/mol	Joback Method
hfus	16.34	kJ/mol	Joback Method
hvap	48.17	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.833		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	1383.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1385.00		NIST Webbook
tb	513.22	K	Joback Method
tc	758.83	K	Joback Method
tf	410.66	K	Joback Method
vc	0.499	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.40	J/molxK	513.22	Joback Method
cpg	330.58	J/molxK	554.15	Joback Method
cpg	345.74	J/molxK	595.09	Joback Method
cpg	359.92	J/molxK	636.02	Joback Method
cpg	373.16	J/molxK	676.96	Joback Method
cpg	385.51	J/molxK	717.89	Joback Method
cpg	397.01	J/molxK	758.83	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=R62186&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R62186&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>
<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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