

# 3-Ethyl-5-methyl-1,2,4-trithiolane

<b>Inchi:</b>	InChI=1S/C5H10S3/c1-3-5-6-4(2)7-8-5/h4-5H,3H2,1-2H3
<b>InchiKey:</b>	SHLIDHGBMLQTDS-UHFFFAOYSA-N
<b>Formula:</b>	C5H10S3
<b>SMILES:</b>	CCC1SSC(C)S1
<b>Mol. weight [g/mol]:</b>	166.33
<b>CAS:</b>	116505-59-0

## Physical Properties

Property code	Value	Unit	Source
gf	139.64	kJ/mol	Joback Method
hf	29.39	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	44.11	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.197		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
rinpol	1217.00		NIST Webbook
rinpol	1255.20		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1255.20		NIST Webbook
tb	467.90	K	Joback Method
tc	717.05	K	Joback Method
tf	403.12	K	Joback Method
vc	0.394	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.19	J/molxK	467.90	Joback Method
cpg	242.52	J/molxK	509.42	Joback Method
cpg	255.01	J/molxK	550.95	Joback Method
cpg	266.70	J/molxK	592.47	Joback Method
cpg	277.61	J/molxK	634.00	Joback Method

cpg	287.79	J/mol×K	675.52	Joback Method
cpg	297.27	J/mol×K	717.05	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=C116505590&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116505590&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>hvap:</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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