

# 3-(ethylthio)-1,2,4-trithiane

Inchi:	InChI=1S/C5H10S4/c1-2-6-5-7-3-4-8-9-5/h5H,2-4H2,1H3
InchiKey:	KIBXTVJUTYQFGB-UHFFFAOYSA-N
Formula:	C5H10S4
SMILES:	CCSC1SCCSS1
Mol. weight [g/mol]:	198.39

## Physical Properties

Property code	Value	Unit	Source
gf	168.37	kJ/mol	Joback Method
hf	85.44	kJ/mol	Joback Method
hfus	15.64	kJ/mol	Joback Method
hvap	51.41	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.151		Crippen Method
mcvol	135.850	ml/mol	McGowan Method
pc	4480.21	kPa	Joback Method
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook
tb	545.62	K	Joback Method
tc	830.41	K	Joback Method
tf	438.24	K	Joback Method
vc	0.441	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.67	J/mol×K	545.62	Joback Method
cpg	286.95	J/mol×K	593.09	Joback Method
cpg	300.12	J/mol×K	640.55	Joback Method
cpg	312.23	J/mol×K	688.02	Joback Method
cpg	323.32	J/mol×K	735.48	Joback Method
cpg	333.41	J/mol×K	782.95	Joback Method
cpg	342.55	J/mol×K	830.41	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=R225780&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R225780&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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