

# 3-Ethylthiane

<b>Other names:</b>	3-Ethyltetrahydro-2H-thiopyran 3-Ethyl-thiacyclohexane
<b>Inchi:</b>	InChI=1S/C7H14S/c1-2-7-4-3-5-8-6-7/h7H,2-6H2,1H3
<b>InchiKey:</b>	CIMHGPVZHGEPEP-UHFFFAOYSA-N
<b>Formula:</b>	C7H14S
<b>SMILES:</b>	CCC1CCCSC1
<b>Mol. weight [g/mol]:</b>	130.25
<b>CAS:</b>	61568-48-7

## Physical Properties

Property code	Value	Unit	Source
gf	72.37	kJ/mol	Joback Method
hf	-88.23	kJ/mol	Joback Method
hfus	9.38	kJ/mol	Joback Method
hvap	37.42	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.540		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
tb	426.94	K	Joback Method
tc	646.42	K	Joback Method
tf	259.48	K	Joback Method
vc	0.406	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.37	J/mol×K	426.94	Joback Method
cpg	236.92	J/mol×K	463.52	Joback Method
cpg	252.59	J/mol×K	500.10	Joback Method
cpg	267.39	J/mol×K	536.68	Joback Method

cpg	281.37	J/mol×K	573.26	Joback Method
cpg	294.54	J/mol×K	609.84	Joback Method
cpg	306.93	J/mol×K	646.42	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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=C61568487&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61568487&amp;Units=SI</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>mvol:</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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