

# trans-2-Ethyl-5-methylthiolane

<b>Other names:</b>	Thiolane, 2-ethyl-5-methyl, trans- trans-5-ethyl-2-methyl-thiacyclopentane
<b>Inchi:</b>	InChI=1S/C7H14S/c1-3-7-5-4-6(2)8-7/h6-7H,3-5H2,1-2H3/t6-,7-/m1/s1
<b>InchiKey:</b>	GLYJMWLDSMBPTO-RNFRBKRXSA-N
<b>Formula:</b>	C7H14S
<b>SMILES:</b>	CCC1CCC(C)S1
<b>Mol. weight [g/mol]:</b>	130.25

## Physical Properties

Property code	Value	Unit	Source
gf	76.76	kJ/mol	Joback Method
hf	-102.41	kJ/mol	Joback Method
hfus	12.55	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.680		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
tb	418.00	K	Joback Method
tc	628.19	K	Joback Method
tf	258.76	K	Joback Method
vc	0.413	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.88	J/molxK	418.00	Joback Method

cpg	237.68	J/mol×K	453.03	Joback Method
cpg	252.69	J/mol×K	488.06	Joback Method
cpg	266.93	J/mol×K	523.09	Joback Method
cpg	280.42	J/mol×K	558.12	Joback Method
cpg	293.20	J/mol×K	593.16	Joback Method
cpg	305.28	J/mol×K	628.19	Joback Method

## Sources

<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=R41708&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R41708&amp;Units=SI</a>
<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>

## 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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