

# cis-2-Ethyl-3-methylthiophane

<b>Other names:</b>	2-Ethyl-3-methyltetrahydrothiophene, cis- cis-2-ethyl-3-methyl-thiacyclopentane Thiophene, 2-ethyltetrahydro-3-methyl-, cis-
<b>Inchi:</b>	InChI=1S/C7H14S/c1-3-7-6(2)4-5-8-7/h6-7H,3-5H2,1-2H3/t6-,7-/m1/s1
<b>InchiKey:</b>	XNZCGHZDGGZDSBU-RNFRBKRXSA-N
<b>Formula:</b>	C7H14S
<b>SMILES:</b>	CCC1SCCC1C
<b>Mol. weight [g/mol]:</b>	130.25
<b>CAS:</b>	61568-37-4

## 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	-2.40		Crippen Method
logp	2.538		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
tb	418.00	K	Joback Method
tc	628.19	K	Joback Method
tf	258.76	K	Joback Method
vc	0.413	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.88	J/mol×K	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

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C61568374&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61568374&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>
<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>

## 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>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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