

# Trans-2,5-dimethylthiane

<b>Other names:</b>	trans-2,5-dimethyl-thiacyclohexane
<b>Inchi:</b>	InChI=1S/C7H14S/c1-6-3-4-7(2)8-5-6/h6-7H,3-5H2,1-2H3/t6-,7-/m0/s1
<b>InchiKey:</b>	FCFFROVETURYHE-BQBZGAKWSA-N
<b>Formula:</b>	C7H14S
<b>SMILES:</b>	CC1CCC(C)SC1
<b>Mol. weight [g/mol]:</b>	130.25

## Physical Properties

Property code	Value	Unit	Source
gf	64.66	kJ/mol	Joback Method
hf	-108.57	kJ/mol	Joback Method
hfus	10.45	kJ/mol	Joback Method
hvap	37.11	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.538		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	901.00		NIST Webbook
rinpol	865.00		NIST Webbook
tb	422.27	K	Joback Method
tc	641.36	K	Joback Method
tf	255.24	K	Joback Method
vc	0.406	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.70	J/mol×K	422.27	Joback Method
cpg	237.55	J/mol×K	458.78	Joback Method
cpg	253.57	J/mol×K	495.30	Joback Method
cpg	268.76	J/mol×K	531.81	Joback Method
cpg	283.14	J/mol×K	568.33	Joback Method
cpg	296.74	J/mol×K	604.84	Joback Method
cpg	309.57	J/mol×K	641.36	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=U215068&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U215068&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>rinpola:</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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