

# trans,cis-2,3,5-trimethyl-thiacyclopentane

<b>Inchi:</b>	InChI=1S/C7H14S/c1-5-4-6(2)8-7(5)3/h5-7H,4H2,1-3H3/t5-,6-,7+/m1/s1
<b>InchiKey:</b>	MLHOTFJTKPLNPX-QYNIQEEDSA-N
<b>Formula:</b>	C7H14S
<b>SMILES:</b>	CC1CC(C)C(C)S1
<b>Mol. weight [g/mol]:</b>	130.25

## Physical Properties

Property code	Value	Unit	Source
gf	69.05	kJ/mol	Joback Method
hf	-122.75	kJ/mol	Joback Method
hfus	13.62	kJ/mol	Joback Method
hvap	36.63	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.536		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpola	941.00		NIST Webbook
tb	413.33	K	Joback Method
tc	623.07	K	Joback Method
tf	254.52	K	Joback Method
vc	0.412	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.18	J/mol×K	413.33	Joback Method
cpg	238.25	J/mol×K	448.29	Joback Method
cpg	253.57	J/mol×K	483.24	Joback Method
cpg	268.15	J/mol×K	518.20	Joback Method
cpg	282.02	J/mol×K	553.16	Joback Method
cpg	295.20	J/mol×K	588.11	Joback Method
cpg	307.68	J/mol×K	623.07	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R209035&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R209035&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>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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