

# Thiocyclohexane, 4-isopropylidene

**Inchi:** InChI=1S/C8H14S/c1-7(2)8-3-5-9-6-4-8/h3-6H2,1-2H3  
**InchiKey:** PQJVJPZYCLILFJ-UHFFFAOYSA-N  
**Formula:** C8H14S  
**SMILES:** CC(C)=C1CCSCC1  
**Mol. weight [g/mol]:** 142.26

## Physical Properties

Property code	Value	Unit	Source
gf	125.41	kJ/mol	Joback Method
hf	-22.29	kJ/mol	Joback Method
hfus	9.91	kJ/mol	Joback Method
hvap	40.82	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.850		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	1121.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1384.00		NIST Webbook
tb	461.01	K	Joback Method
tc	690.65	K	Joback Method
tf	271.39	K	Joback Method
vc	0.448	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.68	J/mol×K	461.01	Joback Method
cpg	263.97	J/mol×K	499.28	Joback Method
cpg	279.26	J/mol×K	537.56	Joback Method
cpg	293.62	J/mol×K	575.83	Joback Method
cpg	307.07	J/mol×K	614.10	Joback Method
cpg	319.67	J/mol×K	652.38	Joback Method
cpg	331.46	J/mol×K	690.65	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R384473&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R384473&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>
<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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	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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