

# 1-Thiacycloheptane,3,3,6,6-tetramethyl-

<b>Inchi:</b>	InChI=1S/C10H20S/c1-9(2)5-6-10(3,4)8-11-7-9/h5-8H2,1-4H3
<b>InchiKey:</b>	KYRUZIUZBMLVTF-UHFFFAOYSA-N
<b>Formula:</b>	C10H20S
<b>SMILES:</b>	CC1(C)CCC(C)(C)CSC1
<b>Mol. weight [g/mol]:</b>	172.33
<b>CAS:</b>	53561-47-0

## Physical Properties

Property code	Value	Unit	Source
gf	66.84	kJ/mol	Joback Method
hf	-146.17	kJ/mol	Joback Method
hfus	3.52	kJ/mol	Joback Method
hvap	41.66	kJ/mol	Joback Method
ie	8.15	eV	NIST Webbook
log10ws	-3.30		Crippen Method
logp	3.566		Crippen Method
mcvol	157.250	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
tb	495.66	K	Joback Method
tc	733.68	K	Joback Method
tf	333.33	K	Joback Method
vc	0.561	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.67	J/molxK	495.66	Joback Method
cpg	375.91	J/molxK	535.33	Joback Method
cpg	395.52	J/molxK	575.00	Joback Method
cpg	413.76	J/molxK	614.67	Joback Method
cpg	430.87	J/molxK	654.34	Joback Method
cpg	447.09	J/molxK	694.01	Joback Method
cpg	462.69	J/molxK	733.68	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=C53561470&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53561470&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>

# 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>ie:</b>	Ionization energy
<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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