

# 2H-Thiapyrane, 2-methyl

<b>Other names:</b>	2-Methyl-2H-thiapyrane 2-methyl-(2H)-thiapyran
<b>Inchi:</b>	InChI=1S/C6H8S/c1-6-4-2-3-5-7-6/h2-6H,1H3
<b>InchiKey:</b>	OYDIECGUBNPZFY-UHFFFAOYSA-N
<b>Formula:</b>	C6H8S
<b>SMILES:</b>	CC1C=CC=CS1
<b>Mol. weight [g/mol]:</b>	112.19

## Physical Properties

Property code	Value	Unit	Source
gf	123.87	kJ/mol	Joback Method
hf	47.97	kJ/mol	Joback Method
hfus	9.23	kJ/mol	Joback Method
hvap	35.78	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.192		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	912.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
ripol	1290.00		NIST Webbook
tb	402.38	K	Joback Method
tc	629.56	K	Joback Method
tf	249.73	K	Joback Method
vc	0.323	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.62	J/mol×K	402.38	Joback Method
cpg	167.00	J/mol×K	440.24	Joback Method
cpg	178.64	J/mol×K	478.11	Joback Method

cpg	189.55	J/mol×K	515.97	Joback Method
cpg	199.77	J/mol×K	553.83	Joback Method
cpg	209.32	J/mol×K	591.70	Joback Method
cpg	218.24	J/mol×K	629.56	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R194686&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R194686&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>rinpol:</b>	Non-polar retention indices
<b>ripol:</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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