

# 2-Propyl-2H-thiapyrane

<b>Inchi:</b>	InChI=1S/C8H12S/c1-2-5-8-6-3-4-7-9-8/h3-4,6-8H,2,5H2,1H3
<b>InchiKey:</b>	DYBCSWILIAFIDP-UHFFFAOYSA-N
<b>Formula:</b>	C8H12S
<b>SMILES:</b>	CCCC1C=CC=CS1
<b>Mol. weight [g/mol]:</b>	140.25

## Physical Properties

Property code	Value	Unit	Source
gf	140.71	kJ/mol	Joback Method
hf	6.69	kJ/mol	Joback Method
hfus	14.41	kJ/mol	Joback Method
hvap	40.23	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.972		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	1117.00		NIST Webbook
rinpol	1117.00		NIST Webbook
ripol	1487.00		NIST Webbook
tb	448.14	K	Joback Method
tc	669.28	K	Joback Method
tf	272.27	K	Joback Method
vc	0.434	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.11	J/molxK	448.14	Joback Method
cpg	248.13	J/molxK	485.00	Joback Method
cpg	262.27	J/molxK	521.85	Joback Method
cpg	275.56	J/molxK	558.71	Joback Method
cpg	288.04	J/molxK	595.57	Joback Method
cpg	299.73	J/molxK	632.43	Joback Method
cpg	310.68	J/molxK	669.28	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R194700&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R194700&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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