

# 2-Acetyl-2,3,5,6-tetrahydro-1,4-thiazine

<b>Inchi:</b>	InChI=1S/C6H11NOS/c1-5(8)6-4-9-3-2-7-6/h6-7H,2-4H2,1H3
<b>InchiKey:</b>	VZWHTXPYIXULDX-UHFFFAOYSA-N
<b>Formula:</b>	C6H11NOS
<b>SMILES:</b>	CC(=O)C1CSCCN1
<b>Mol. weight [g/mol]:</b>	145.22

## Physical Properties

Property code	Value	Unit	Source
gf	22.74	kJ/mol	Joback Method
hf	-142.36	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	48.69	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	0.280		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
rinpola	1225.00		NIST Webbook
tb	506.48	K	Joback Method
tc	747.62	K	Joback Method
tf	403.17	K	Joback Method
vc	0.394	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.64	J/mol×K	506.48	Joback Method
cpg	253.08	J/mol×K	546.67	Joback Method
cpg	266.67	J/mol×K	586.86	Joback Method
cpg	279.42	J/mol×K	627.05	Joback Method
cpg	291.36	J/mol×K	667.24	Joback Method
cpg	302.48	J/mol×K	707.43	Joback Method
cpg	312.82	J/mol×K	747.62	Joback Method

# Sources

<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=U281473&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U281473&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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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