

# 2-Propionyl-2-thiazoline

<b>Inchi:</b>	InChI=1S/C6H9NOS/c1-2-5(8)6-7-3-4-9-6/h2-4H2,1H3
<b>InchiKey:</b>	MFQABLFJUQNPAC-UHFFFAOYSA-N
<b>Formula:</b>	C6H9NOS
<b>SMILES:</b>	CCC(=O)C1=NCCS1
<b>Mol. weight [g/mol]:</b>	143.21

## Physical Properties

Property code	Value	Unit	Source
gf	91.95	kJ/mol	Joback Method
hf	-36.39	kJ/mol	Joback Method
hfus	15.39	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.111		Crippen Method
mcvol	108.140	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
rinpol	1196.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1205.00		NIST Webbook
ripol	1850.00		NIST Webbook
ripol	1803.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1850.00		NIST Webbook
tb	516.17	K	Joback Method
tc	756.55	K	Joback Method
tf	390.72	K	Joback Method
vc	0.401	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	235.98	J/mol×K	516.17	Joback Method
cpg	248.87	J/mol×K	556.23	Joback Method
cpg	260.95	J/mol×K	596.30	Joback Method
cpg	272.22	J/mol×K	636.36	Joback Method
cpg	282.72	J/mol×K	676.43	Joback Method
cpg	292.46	J/mol×K	716.49	Joback Method
cpg	301.46	J/mol×K	756.55	Joback Method

## Sources

<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>
<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=R225562&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R225562&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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