

# 2-((Z)-2-butenyl)thiazolidine

<b>Inchi:</b>	InChI=1S/C7H13NS/c1-2-3-4-7-8-5-6-9-7/h2-3,7-8H,4-6H2,1H3/b3-2-
<b>InchiKey:</b>	NVCZSVLOACZRHY-IHWYPQMZSA-N
<b>Formula:</b>	C7H13NS
<b>SMILES:</b>	CC=CCC1NCCS1
<b>Mol. weight [g/mol]:</b>	143.25

## Physical Properties

Property code	Value	Unit	Source
gf	252.40	kJ/mol	Joback Method
hf	72.96	kJ/mol	Joback Method
hfus	21.27	kJ/mol	Joback Method
hvap	43.96	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.615		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
tb	475.38	K	Joback Method
tc	704.29	K	Joback Method
tf	362.95	K	Joback Method
vc	0.431	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.70	J/mol×K	475.38	Joback Method
cpg	261.96	J/mol×K	513.53	Joback Method
cpg	276.29	J/mol×K	551.68	Joback Method
cpg	289.75	J/mol×K	589.83	Joback Method
cpg	302.36	J/mol×K	627.99	Joback Method
cpg	314.19	J/mol×K	666.14	Joback Method
cpg	325.27	J/mol×K	704.29	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R163627&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R163627&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>hvpap:</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>rinppl:</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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