

# 2-nonylthiazolidine

<b>Inchi:</b>	InChI=1S/C12H25NS/c1-2-3-4-5-6-7-8-9-12-13-10-11-14-12/h12-13H,2-11H2,1H3
<b>InchiKey:</b>	DOTWLKBBHRRWHT-UHFFFAOYSA-N
<b>Formula:</b>	C12H25NS
<b>SMILES:</b>	CCCCCCCCC1NCCS1
<b>Mol. weight [g/mol]:</b>	215.40
<b>CAS:</b>	116112-94-8

## Physical Properties

Property code	Value	Unit	Source
gf	214.28	kJ/mol	Joback Method
hf	-147.46	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	55.13	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.790		Crippen Method
mvol	195.410	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1722.00		NIST Webbook
tb	585.62	K	Joback Method
tc	787.28	K	Joback Method
tf	424.38	K	Joback Method
vc	0.732	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.28	J/molxK	585.62	Joback Method
cpg	521.64	J/molxK	619.23	Joback Method
cpg	539.99	J/molxK	652.84	Joback Method
cpg	557.38	J/molxK	686.45	Joback Method
cpg	573.84	J/molxK	720.06	Joback Method
cpg	589.40	J/molxK	753.67	Joback Method
cpg	604.10	J/molxK	787.28	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C116112948&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116112948&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>hvp:</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>rinp:</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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