

# 2,4-Dimethyl-3-thiazoline

Inchi:	InChI=1S/C5H9NS/c1-4-3-6-5(2)7-4/h3-5H,1-2H3
InchiKey:	VPUJUMSZUQCZNQ-UHFFFAOYSA-N
Formula:	C5H9NS
SMILES:	CC1C=NC(C)S1
Mol. weight [g/mol]:	115.20

## Physical Properties

Property code	Value	Unit	Source
gf	206.66	kJ/mol	Joback Method
hf	67.62	kJ/mol	Joback Method
hfus	13.73	kJ/mol	Joback Method
hvap	38.99	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.538		Crippen Method
mcvol	92.480	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
rinpol	962.00		NIST Webbook
rinpol	975.00		NIST Webbook
ripol	1425.00		NIST Webbook
tb	425.10	K	Joback Method
tc	656.38	K	Joback Method
tf	308.52	K	Joback Method
vc	0.337	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.69	J/molxK	425.10	Joback Method
cpg	194.56	J/molxK	463.65	Joback Method
cpg	207.73	J/molxK	502.19	Joback Method
cpg	220.21	J/molxK	540.74	Joback Method
cpg	232.00	J/molxK	579.29	Joback Method
cpg	243.10	J/molxK	617.84	Joback Method
cpg	253.52	J/molxK	656.38	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=R282649&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R282649&amp;Units=SI</a>
<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>

# 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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