

# 4,5-dimethyl-2-isobutyl-3-thiazoline, trans

Inchi:	InChI=1S/C9H17NS/c1-6(2)5-9-10-7(3)8(4)11-9/h6,8-9H,5H2,1-4H3/t8-,9-/m0/s1
InchiKey:	FDOISHJOXPONIV-IUCAKERBSA-N
Formula:	C9H17NS
SMILES:	CC1=NC(CC(C)C)SC1C
Mol. weight [g/mol]:	171.30

## Physical Properties

Property code	Value	Unit	Source
gf	228.27	kJ/mol	Joback Method
hf	-31.69	kJ/mol	Joback Method
hfus	20.18	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.955		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	1256.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
ripol	1612.00		NIST Webbook
tb	521.16	K	Joback Method
tc	744.46	K	Joback Method
tf	351.12	K	Joback Method
vc	0.554	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.44	J/molxK	521.16	Joback Method
cpg	372.87	J/molxK	558.38	Joback Method
cpg	390.33	J/molxK	595.59	Joback Method
cpg	406.83	J/molxK	632.81	Joback Method
cpg	422.40	J/molxK	670.03	Joback Method
cpg	437.03	J/molxK	707.25	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R497722&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R497722&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>
<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>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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