

# 5-ethyl-4-methyl-2-octyl-3-thiazoline, cis

<b>Inchi:</b>	InChI=1S/C14H27NS/c1-4-6-7-8-9-10-11-14-15-12(3)13(5-2)16-14/h13-14H,4-11H2,1-3H
<b>InchiKey:</b>	OODRCQYLMQGWMM-KGLIPLIRSA-N
<b>Formula:</b>	C14H27NS
<b>SMILES:</b>	CCCCCCCC1N=C(C)C(CC)S1
<b>Mol. weight [g/mol]:</b>	241.44

## Physical Properties

Property code	Value	Unit	Source
gf	272.81	kJ/mol	Joback Method
hf	-129.61	kJ/mol	Joback Method
hfus	36.65	kJ/mol	Joback Method
hvap	59.68	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.049		Crippen Method
mcvol	219.290	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	1802.00		NIST Webbook
rinpol	1797.00		NIST Webbook
ripol	2179.00		NIST Webbook
tb	636.00	K	Joback Method
tc	837.66	K	Joback Method
tf	422.47	K	Joback Method
vc	0.841	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.38	J/molxK	636.00	Joback Method
cpg	630.96	J/molxK	669.61	Joback Method
cpg	650.43	J/molxK	703.22	Joback Method
cpg	668.83	J/molxK	736.83	Joback Method
cpg	686.18	J/molxK	770.44	Joback Method
cpg	702.50	J/molxK	804.05	Joback Method
cpg	717.80	J/molxK	837.66	Joback Method

# Sources

<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=R498314&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R498314&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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