

# 2-octyl-4-methyl-3-thiazoline

<b>Other names:</b>	4-methyl-2-octyl-3-thiazoline
<b>Inchi:</b>	InChI=1S/C12H23NS/c1-3-4-5-6-7-8-9-12-13-11(2)10-14-12/h12H,3-10H2,1-2H3
<b>InchiKey:</b>	BVJQPECTWJHPSN-UHFFFAOYSA-N
<b>Formula:</b>	C12H23NS
<b>SMILES:</b>	CCCCCCCCC1N=C(C)CS1
<b>Mol. weight [g/mol]:</b>	213.38

## Physical Properties

Property code	Value	Unit	Source
gf	263.68	kJ/mol	Joback Method
hf	-67.99	kJ/mol	Joback Method
hfus	30.40	kJ/mol	Joback Method
hvap	55.54	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.271		Crippen Method
mcvol	191.110	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1699.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1683.00		NIST Webbook
ripol	2138.00		NIST Webbook
ripol	2138.00		NIST Webbook
tb	594.91	K	Joback Method
tc	802.71	K	Joback Method
tf	404.17	K	Joback Method
vc	0.730	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.14	J/mol×K	594.91	Joback Method
cpg	521.50	J/mol×K	629.54	Joback Method
cpg	539.82	J/mol×K	664.18	Joback Method

cpg	557.13	J/mol×K	698.81	Joback Method
cpg	573.43	J/mol×K	733.44	Joback Method
cpg	588.77	J/mol×K	768.08	Joback Method
cpg	603.17	J/mol×K	802.71	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R230905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R230905&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>

## 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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