

# 2-Methyl-4-isopropyl-delta<sup>2</sup>-thiazoline

<b>Other names:</b>	2-Methyl-4-isopropyl-delta
<b>Inchi:</b>	InChI=1S/C7H13NS/c1-5(2)7-4-9-6(3)8-7/h5,7H,4H2,1-3H3
<b>InchiKey:</b>	DYMRFOBZZQTGRL-UHFFFAOYSA-N
<b>Formula:</b>	C7H13NS
<b>SMILES:</b>	CC1=NC(C(C)C)CS1
<b>Mol. weight [g/mol]:</b>	143.25
<b>CAS:</b>	4146-21-8

## Physical Properties

Property code	Value	Unit	Source
gf	219.14	kJ/mol	Joback Method
hf	29.93	kJ/mol	Joback Method
hfus	13.93	kJ/mol	Joback Method
hvap	44.02	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.176		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
tb	480.07	K	Joback Method
tc	711.48	K	Joback Method
tf	332.82	K	Joback Method
vc	0.444	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.14	J/molxK	480.07	Joback Method
cpg	279.21	J/molxK	518.64	Joback Method
cpg	294.41	J/molxK	557.21	Joback Method
cpg	308.75	J/molxK	595.77	Joback Method
cpg	322.25	J/molxK	634.34	Joback Method
cpg	334.93	J/molxK	672.91	Joback Method
cpg	346.78	J/molxK	711.48	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=C4146218&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4146218&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>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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