

# 2,4,4-Trimethyl-delta<sup>2</sup>-thiazoline

<b>Other names:</b>	2,4,4-Trimethyl-delta
<b>Inchi:</b>	InChI=1S/C6H11NS/c1-5-7-6(2,3)4-8-5/h4H2,1-3H3
<b>InchiKey:</b>	RHYWBMKYLKNBET-UHFFFAOYSA-N
<b>Formula:</b>	C6H11NS
<b>SMILES:</b>	CC1=NC(C)(C)CS1
<b>Mol. weight [g/mol]:</b>	129.22
<b>CAS:</b>	4145-94-2

## Physical Properties

Property code	Value	Unit	Source
gf	207.67	kJ/mol	Joback Method
hf	71.09	kJ/mol	Joback Method
hfus	8.56	kJ/mol	Joback Method
hvap	41.03	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.930		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4146.27	kPa	Joback Method
tb	457.87	K	Joback Method
tc	698.22	K	Joback Method
tf	360.45	K	Joback Method
vc	0.392	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.48	J/molxK	457.87	Joback Method
cpg	236.01	J/molxK	497.93	Joback Method
cpg	249.45	J/molxK	537.99	Joback Method
cpg	261.91	J/molxK	578.05	Joback Method
cpg	273.54	J/molxK	618.11	Joback Method
cpg	284.44	J/molxK	658.16	Joback Method
cpg	294.75	J/molxK	698.22	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=C4145942&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4145942&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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/32-045-6/2-4-4-Trimethyl-delta-2-thiazoline.pdf>

Generated by Cheméo on 2024-04-29 12:51:56.958141751 +0000 UTC m=+16684365.878719111.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.