

# 2-butyl-5-ethyl-4-methyl-3-thiazoline, trans

<b>Inchi:</b>	InChI=1S/C10H19NS/c1-4-6-7-10-11-8(3)9(5-2)12-10/h9-10H,4-7H2,1-3H3/t9-,10-/m0/s1
<b>InchiKey:</b>	KKDDEAQGACNGDN-UWVGGRQHSA-N
<b>Formula:</b>	C10H19NS
<b>SMILES:</b>	CCCCC1N=C(C)C(CC)S1
<b>Mol. weight [g/mol]:</b>	185.33

## Physical Properties

Property code	Value	Unit	Source
gf	239.13	kJ/mol	Joback Method
hf	-47.05	kJ/mol	Joback Method
hfus	26.29	kJ/mol	Joback Method
hvap	50.78	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.489		Crippen Method
mcvol	162.930	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinqol	1395.00		NIST Webbook
tb	544.48	K	Joback Method
tc	759.10	K	Joback Method
tf	377.39	K	Joback Method
vc	0.617	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.20	J/mol×K	544.48	Joback Method
cpg	420.89	J/mol×K	580.25	Joback Method
cpg	438.62	J/mol×K	616.02	Joback Method
cpg	455.40	J/mol×K	651.79	Joback Method
cpg	471.25	J/mol×K	687.56	Joback Method
cpg	486.18	J/mol×K	723.33	Joback Method
cpg	500.19	J/mol×K	759.10	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=R497544&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R497544&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>

# 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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-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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