

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

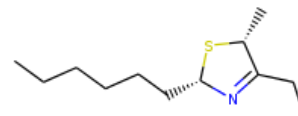
**InChI:** InChI=1S/C12H23NS/c1-4-6-7-8-9-12-13-11(5-2)10(3)14-12/h10,12H,4-9H2,1-3H3/t10-,12+/m1/s1

**InChI Key:** YNMIAYYDICMIHA-PWSUYJOCSA-N

**Formula:** C<sub>12</sub>H<sub>23</sub>NS

**SMILES:** CCCCCC1N=C(CC)C(C)S1

**Molecular Weight:** 213.38



## Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	255.97	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-88.33	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	31.47	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	55.23	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.27		Crippen Method
$P_c$	2053.03	kPa	Joback Method
$T_{\text{boil}}$	590.24	K	Joback Method
$T_c$	797.96	K	Joback Method
$T_{\text{fus}}$	399.93	K	Joback Method
$V_c$	0.73	m <sup>3</sup> /kg-mol	Joback Method

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	503.26	J/mol×K	590.24	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H23NS/c1-4-6-7-8-9-12-13-11\(5-2\)10\(3\)14-12/h10,12H,4-9H2,1-3H3/t10-,12+/m1/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H23NS/c1-4-6-7-8-9-12-13-11(5-2)10(3)14-12/h10,12H,4-9H2,1-3H3/t10-,12+/m1/s1)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$C_{p, gas}$ : Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{oct/wat}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

$T_{boil}$ : Normal Boiling Point Temperature (K).

$T_c$ : Critical Temperature (K).

$T_{fus}$ : Normal melting (fusion) point (K).

$V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

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