

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

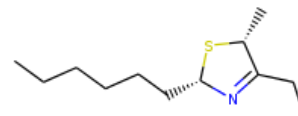
InChI: InChI=1S/C12H23NS/c1-4-6-7-8-9-12-13-11(5-2)10(3)14-12/h10,12H,4-9H2,1-3H3/t10-,12+/m1/s1

InChI Key: YNMIAYYDICMIHA-PWSUYJOCSA-N

Formula: C₁₂H₂₃NS

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
$\log P_{\text{oct/wat}}$	4.269		Crippen Method
P_c	2053.03	kPa	Joback Method
T_{boil}	590.24	K	Joback Method
T_c	797.96	K	Joback Method
T_{fus}	399.93	K	Joback Method
V_c	0.729	m ³ /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

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/ci990307l>

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 (m³/kg-mol).

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