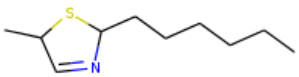
2-hexyl-5-methyl-3-thiazoline

InChI: InChI=1S/C10H19NS/c1-3-4-5-6-7-10-11-8-9(2)12-10/h8-10H,3-7H2,1-2H3
InChI Key: DFENOVAXGLVQNZ-UHFFFAOYSA-N
Formula: C10H19NS
SMILES: CCCCCCC1N=CC(C)S1
Molecular Weight: 185.33



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	248.76	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-35.58	kJ/mol	Joback Method
$\Delta_{fus} H°$	26.68	kJ/mol	Joback Method
$\Delta_{vap} H°$	50.12	kJ/mol	Joback Method
$logP_{oct/wat}$	3.49		Crippen Method
P_c	2500.00	kPa	Joback Method
T_{boil}	539.50	K	Joback Method
T_c	753.02	K	Joback Method
T_{fus}	364.87	K	Joback Method
V_c	0.62	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	401.71	J/mol×K	539.5	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H19NS/c1-3-4-5-6-7-10-11-8-9(2)12-10/h8-10H,3-7H2,1-2H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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^3/kg-mol).