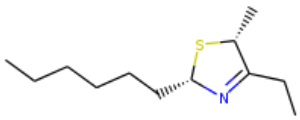
4-ethyl-2-hexyl-5-methyl-3-thiazoline, cis

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: CCCCCCC1N=C(CC)C(C)S1
Molecular Weight: 213.38



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	255.97	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-88.33	kJ/mol	Joback Method
$\Delta_{fus} H°$	31.47	kJ/mol	Joback Method
$\Delta_{vap} H°$	55.23	kJ/mol	Joback Method
$logP_{oct/wat}$	4.27		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	0.73	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	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

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).

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