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-,1
InchiKey: YNMIAYYDICMIHA-PWSUYJOCSA-N
Formula: C12H23NS
SMILES: CCCCCCC1N=C(CC)C(C)S1
Mol. weight [g/mol]: 213.38

Physical Properties

Property code	Value	Unit	Source
gf	255.97	kJ/mol	Joback Method
hf	-88.33	kJ/mol	Joback Method
hfus	31.47	kJ/mol	Joback Method
hvap	55.23	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.269		Crippen Method
mcvol	191.110	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1569.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1569.00		NIST Webbook
ripol	1905.00		NIST Webbook
ripol	1905.00		NIST Webbook
tb	590.24	K	Joback Method
tc	797.96	K	Joback Method
tf	399.93	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.26	J/mol×K	590.24	Joback Method
cpg	523.09	J/mol×K	624.86	Joback Method
cpg	541.88	J/mol×K	659.48	Joback Method
cpg	559.65	J/mol×K	694.10	Joback Method
cpg	576.42	J/mol×K	728.72	Joback Method

cpg	592.19	J/mol×K	763.34	Joback Method
cpg	607.00	J/mol×K	797.96	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497900&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume