4-ethyl-5-methyl-2-pentyl-3-thiazoline, trans

Inchi: InChI=1S/C11H21NS/c1-4-6-7-8-11-12-10(5-2)9(3)13-11/h9,11H,4-8H2,1-3H3/t9-,11-/m0
InchiKey: ZHVXHJIJBSMTDB-ONGXEEELSA-N
Formula: C11H21NS
SMILES: CCCCCC1N=C(CC)C(C)S1
Mol. weight [g/mol]: 199.36

Physical Properties

Property code	Value	Unit	Source
gf	247.55	kJ/mol	Joback Method
hf	-67.69	kJ/mol	Joback Method
hfus	28.88	kJ/mol	Joback Method
hvap	53.00	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.879		Crippen Method
mcvol	177.020	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1477.00		NIST Webbook
ripol	1816.00		NIST Webbook
tb	567.36	K	Joback Method
tc	778.45	K	Joback Method
tf	388.66	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.92	J/mol×K	567.36	Joback Method
cpg	471.24	J/mol×K	602.54	Joback Method
cpg	489.55	J/mol×K	637.72	Joback Method
cpg	506.88	J/mol×K	672.90	Joback Method
cpg	523.23	J/mol×K	708.09	Joback Method
cpg	538.63	J/mol×K	743.27	Joback Method
cpg	553.08	J/mol×K	778.45	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=R498087&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