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

Inchi: InChI=1S/C9H17NS/c1-3-4-5-6-9-10-7-8(2)11-9/h7-9H,3-6H2,1-2H3/t8-,9-/m0/s1
InchiKey: RNXFXLBWILWRDA-IUCAKERBSA-N
Formula: C9H17NS
SMILES: CCCCCC1N=CC(C)S1
Mol. weight [g/mol]: 171.30

Physical Properties

Property code	Value	Unit	Source
gf	240.34	kJ/mol	Joback Method
hf	-14.94	kJ/mol	Joback Method
hfus	24.09	kJ/mol	Joback Method
hvap	47.89	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.099		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1345.00		NIST Webbook
tb	516.62	K	Joback Method
tc	733.72	K	Joback Method
tf	353.60	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.65	J/mol×K	516.62	Joback Method
cpg	371.94	J/mol×K	552.80	Joback Method
cpg	389.27	J/mol×K	588.99	Joback Method
cpg	405.64	J/mol×K	625.17	Joback Method
cpg	421.08	J/mol×K	661.35	Joback Method
cpg	435.60	J/mol×K	697.54	Joback Method
cpg	449.22	J/mol×K	733.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R498394&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume