2-heptyl-5-methyl-3-thiazoline

Inchi: InChI=1S/C11H21NS/c1-3-4-5-6-7-8-11-12-9-10(2)13-11/h9-11H,3-8H2,1-2H3
InchiKey: QIBGKHRNAJELGS-UHFFFAOYSA-N
Formula: C11H21NS
SMILES: CCCCCCCC1N=CC(C)S1
Mol. weight [g/mol]: 199.36

Physical Properties

Property code	Value	Unit	Source
gf	257.18	kJ/mol	Joback Method
hf	-56.22	kJ/mol	Joback Method
hfus	29.27	kJ/mol	Joback Method
hvap	52.34	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.879		Crippen Method
mcvol	177.020	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1558.00		NIST Webbook
rinpol	1558.00		NIST Webbook
tb	562.38	K	Joback Method
tc	772.43	K	Joback Method
tf	376.14	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.48	J/mol×K	562.38	Joback Method
cpg	471.09	J/mol×K	597.39	Joback Method
cpg	489.65	J/mol×K	632.40	Joback Method
cpg	507.18	J/mol×K	667.41	Joback Method
cpg	523.70	J/mol×K	702.42	Joback Method
cpg	539.23	J/mol×K	737.43	Joback Method
cpg	553.80	J/mol×K	772.43	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=R497599&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