4,5-dimethyl-2-pentyl-3-thiazoline, cis

Inchi: InChI=1S/C10H19NS/c1-4-5-6-7-10-11-8(2)9(3)12-10/h9-10H,4-7H2,1-3H3/t9-,10+/m1/s1
InchiKey: GBAKIVDQFZQMSK-ZJUUUORDSA-N
Formula: C10H19NS
SMILES: CCCCCC1N=C(C)C(C)S1
Mol. weight [g/mol]: 185.33

Physical Properties

Property code	Value	Unit	Source
gf	239.13	kJ/mol	Joback Method
hf	-47.05	kJ/mol	Joback Method
hfus	26.29	kJ/mol	Joback Method
hvap	50.78	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.489		Crippen Method
mcvol	162.930	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1397.00		NIST Webbook
rinpol	1401.00		NIST Webbook
ripol	1773.00		NIST Webbook
ripol	1773.00		NIST Webbook
tb	544.48	K	Joback Method
tc	759.10	K	Joback Method
tf	377.39	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.20	J/mol×K	544.48	Joback Method
cpg	420.89	J/mol×K	580.25	Joback Method
cpg	438.62	J/mol×K	616.02	Joback Method
cpg	455.40	J/mol×K	651.79	Joback Method
cpg	471.25	J/mol×K	687.56	Joback Method
cpg	486.18	J/mol×K	723.33	Joback Method

cpg	500.19	J/mol×K	759.10	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=R497811&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume