4,5-dimethyl-2-(1-octenyl)-3-thiazoline, cis

Inchi: InChI=1S/C13H23NS/c1-4-5-6-7-8-9-10-13-14-11(2)12(3)15-13/h9-10,12-13H,4-8H2,1-3
InchiKey: DWHWYFMGINVMJL-GBYBRZQVSA-N
Formula: C13H23NS
SMILES: CCCCCCC=CC1N=C(C)C(C)S1
Mol. weight [g/mol]: 225.39

Physical Properties

Property code	Value	Unit	Source
gf	344.61	kJ/mol	Joback Method
hf	8.25	kJ/mol	Joback Method
hfus	34.26	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.435		Crippen Method
mcvol	200.900	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1696.00		NIST Webbook
rinpol	1696.00		NIST Webbook
tb	617.28	K	Joback Method
tc	830.26	K	Joback Method
tf	406.12	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.02	J/mol×K	617.28	Joback Method
cpg	555.91	J/mol×K	652.78	Joback Method
cpg	574.66	J/mol×K	688.27	Joback Method
cpg	592.31	J/mol×K	723.77	Joback Method
cpg	608.90	J/mol×K	759.27	Joback Method
cpg	624.46	J/mol×K	794.77	Joback Method
cpg	639.03	J/mol×K	830.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497633&Units=SI
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

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