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

Inchi: InChI=1S/C13H21NS/c1-4-5-6-7-8-9-10-13-14-11(2)12(3)15-13/h7-10,12-13H,4-6H2,1-3
InchiKey: DLSYFVPFFOKHTD-GIGCSKJXSA-N
Formula: C13H21NS
SMILES: CCCCC=CC=CC1N=C(C)C(C)S1
Mol. weight [g/mol]: 223.38

Physical Properties

Property code	Value	Unit	Source
gf	424.83	kJ/mol	Joback Method
hf	125.47	kJ/mol	Joback Method
hfus	34.46	kJ/mol	Joback Method
hvap	57.37	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.211		Crippen Method
mcvol	196.600	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1777.00		NIST Webbook
tb	621.44	K	Joback Method
tc	843.40	K	Joback Method
tf	401.04	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.67	J/mol×K	621.44	Joback Method
cpg	535.16	J/mol×K	658.43	Joback Method
cpg	553.44	J/mol×K	695.43	Joback Method
cpg	570.59	J/mol×K	732.42	Joback Method
cpg	586.64	J/mol×K	769.41	Joback Method
cpg	601.65	J/mol×K	806.40	Joback Method
cpg	615.68	J/mol×K	843.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497480&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

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