5-methyl-2-octyl-3-thiazoline

Inchi: InChI=1S/C12H23NS/c1-3-4-5-6-7-8-9-12-13-10-11(2)14-12/h10-12H,3-9H2,1-2H3
InchiKey: NQYROUZZKFVEBU-UHFFFAOYSA-N
Formula: C12H23NS
SMILES: CCCCCCCCC1N=CC(C)S1
Mol. weight [g/mol]: 213.38

Physical Properties

Property code	Value	Unit	Source
gf	265.60	kJ/mol	Joback Method
hf	-76.86	kJ/mol	Joback Method
hfus	31.86	kJ/mol	Joback Method
hvap	54.57	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.269		Crippen Method
mcvol	191.110	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1669.00		NIST Webbook
rinpol	1669.00		NIST Webbook
tb	585.26	K	Joback Method
tc	792.00	K	Joback Method
tf	387.41	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.86	J/mol×K	585.26	Joback Method
cpg	522.95	J/mol×K	619.72	Joback Method
cpg	541.96	J/mol×K	654.17	Joback Method
cpg	559.91	J/mol×K	688.63	Joback Method
cpg	576.83	J/mol×K	723.09	Joback Method
cpg	592.73	J/mol×K	757.54	Joback Method
cpg	607.65	J/mol×K	792.00	Joback Method

Sources

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=R498374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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