2-octyl-4-ethyl-5-methyl-3-thiazoline

Inchi: InChI=1S/C14H27NS/c1-4-6-7-8-9-10-11-14-15-13(5-2)12(3)16-14/h12,14H,4-11H2,1-3H
InchiKey: MHDROSFBIWDYEP-UHFFFAOYSA-N
Formula: C14H27NS
SMILES: CCCCCCCCC1N=C(CC)C(C)S1
Mol. weight [g/mol]: 241.44

Physical Properties

Property code	Value	Unit	Source
gf	272.81	kJ/mol	Joback Method
hf	-129.61	kJ/mol	Joback Method
hfus	36.65	kJ/mol	Joback Method
hvap	59.68	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.049		Crippen Method
mcvol	219.290	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	1769.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1783.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	636.00	K	Joback Method
tc	837.66	K	Joback Method
tf	422.47	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.38	J/mol×K	636.00	Joback Method
cpg	630.96	J/mol×K	669.61	Joback Method
cpg	650.43	J/mol×K	703.22	Joback Method
cpg	668.83	J/mol×K	736.83	Joback Method
cpg	686.18	J/mol×K	770.44	Joback Method

cpg	702.50	J/mol×K	804.05	Joback Method
cpg	717.80	J/mol×K	837.66	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=R230841&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