2-octyl-4-ethyl-3-thiazoline

Inchi: InChI=1S/C13H25NS/c1-3-5-6-7-8-9-10-13-14-12(4-2)11-15-13/h12H,3-11H2,1-2H3
InchiKey: VVCIEZWCKNCURL-UHFFFAOYSA-N
Formula: C13H25NS
SMILES: CCCCCCCCC1=NC(CC)CS1
Mol. weight [g/mol]: 227.41

Physical Properties

Property code	Value	Unit	Source
gf	272.10	kJ/mol	Joback Method
hf	-88.63	kJ/mol	Joback Method
hfus	32.99	kJ/mol	Joback Method
hvap	57.77	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.661		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1770.00		NIST Webbook
ripol	2175.00		NIST Webbook
tb	617.79	K	Joback Method
tc	822.44	K	Joback Method
tf	415.44	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.87	J/mol×K	617.79	Joback Method
cpg	574.64	J/mol×K	651.90	Joback Method
cpg	593.35	J/mol×K	686.01	Joback Method
cpg	611.01	J/mol×K	720.11	Joback Method
cpg	627.65	J/mol×K	754.22	Joback Method
cpg	643.31	J/mol×K	788.33	Joback Method
cpg	658.00	J/mol×K	822.44	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=R330020&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume