4-ethyl-5-methyl-2-nonyl-3-thiazoline, trans

Inchi: InChI=1S/C15H29NS/c1-4-6-7-8-9-10-11-12-15-16-14(5-2)13(3)17-15/h13,15H,4-12H2,1
InchiKey: YTQOHMULGJNNJJ-ZFWWWQNUSA-N
Formula: C15H29NS
SMILES: CCCCCCCCCC1N=C(CC)C(C)S1
Mol. weight [g/mol]: 255.46

Physical Properties

Property code	Value	Unit	Source
gf	281.23	kJ/mol	Joback Method
hf	-150.25	kJ/mol	Joback Method
hfus	39.24	kJ/mol	Joback Method
hvap	61.91	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.439		Crippen Method
mcvol	233.380	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1895.00		NIST Webbook
tb	658.88	K	Joback Method
tc	857.96	K	Joback Method
tf	433.74	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.98	J/mol×K	658.88	Joback Method
cpg	686.81	J/mol×K	692.06	Joback Method
cpg	706.52	J/mol×K	725.24	Joback Method
cpg	725.14	J/mol×K	758.42	Joback Method
cpg	742.68	J/mol×K	791.60	Joback Method
cpg	759.17	J/mol×K	824.78	Joback Method
cpg	774.63	J/mol×K	857.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R498027&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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