2-((Z)-2-hexenyl)thiazolidine

Inchi: InChI=1S/C9H17NS/c1-2-3-4-5-6-9-10-7-8-11-9/h4-5,9-10H,2-3,6-8H2,1H3/b5-4-
InchiKey: GYYGBEACGNYVBC-PLNGDYQASA-N
Formula: C9H17NS
SMILES: CCCC=CCC1NCCS1
Mol. weight [g/mol]: 171.30

Physical Properties

Property code	Value	Unit	Source
gf	269.24	kJ/mol	Joback Method
hf	31.68	kJ/mol	Joback Method
hfus	26.45	kJ/mol	Joback Method
hvap	48.41	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.395		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1381.00		NIST Webbook
tb	521.14	K	Joback Method
tc	742.34	K	Joback Method
tf	385.49	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.91	J/mol×K	521.14	Joback Method
cpg	353.05	J/mol×K	558.01	Joback Method
cpg	369.18	J/mol×K	594.87	Joback Method
cpg	384.35	J/mol×K	631.74	Joback Method
cpg	398.62	J/mol×K	668.61	Joback Method
cpg	412.03	J/mol×K	705.48	Joback Method
cpg	424.62	J/mol×K	742.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R163647&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