2-((Z)-2-octenyl)thiazolidine

Inchi: InChI=1S/C11H21NS/c1-2-3-4-5-6-7-8-11-12-9-10-13-11/h6-7,11-12H,2-5,8-10H2,1H3/b
InchiKey: TWIKNBZHELKJGO-SREVYHEPSA-N
Formula: C11H21NS
SMILES: CCCCCC=CCC1NCCS1
Mol. weight [g/mol]: 199.36

Physical Properties

Property code	Value	Unit	Source
gf	286.08	kJ/mol	Joback Method
hf	-9.60	kJ/mol	Joback Method
hfus	31.63	kJ/mol	Joback Method
hvap	52.86	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.176		Crippen Method
mcvol	177.020	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1589.00		NIST Webbook
rinpol	1589.00		NIST Webbook
tb	566.90	K	Joback Method
tc	780.63	K	Joback Method
tf	408.03	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.29	J/mol×K	566.90	Joback Method
cpg	450.77	J/mol×K	602.52	Joback Method
cpg	468.20	J/mol×K	638.14	Joback Method
cpg	484.63	J/mol×K	673.77	Joback Method
cpg	500.11	J/mol×K	709.39	Joback Method
cpg	514.69	J/mol×K	745.01	Joback Method
cpg	528.41	J/mol×K	780.63	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=R163652&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