2-((Z)-2-heptenyl)thiazolidine

Inchi: InChI=1S/C10H19NS/c1-2-3-4-5-6-7-10-11-8-9-12-10/h5-6,10-11H,2-4,7-9H2,1H3/b6-5-
InchiKey: OUYJEVNIDRWBEJ-WAYWQWQTSA-N
Formula: C10H19NS
SMILES: CCCCC=CCC1NCCS1
Mol. weight [g/mol]: 185.33

Physical Properties

Property code	Value	Unit	Source
gf	277.66	kJ/mol	Joback Method
hf	11.04	kJ/mol	Joback Method
hfus	29.04	kJ/mol	Joback Method
hvap	50.64	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.785		Crippen Method
mcvol	162.930	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	544.02	K	Joback Method
tc	761.43	K	Joback Method
tf	396.76	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.25	J/mol×K	544.02	Joback Method
cpg	401.12	J/mol×K	580.26	Joback Method
cpg	417.96	J/mol×K	616.49	Joback Method
cpg	433.82	J/mol×K	652.73	Joback Method
cpg	448.74	J/mol×K	688.96	Joback Method
cpg	462.78	J/mol×K	725.20	Joback Method
cpg	475.98	J/mol×K	761.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R163632&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

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