2-(1-methylpropyl)thiazolidine

Inchi: InChI=1S/C7H15NS/c1-3-6(2)7-8-4-5-9-7/h6-8H,3-5H2,1-2H3
InchiKey: FIEBNWSCVQZSGR-UHFFFAOYSA-N
Formula: C7H15NS
SMILES: CCC(C)C1NCCS1
Mol. weight [g/mol]: 145.27

Physical Properties

Property code	Value	Unit	Source
gf	169.74	kJ/mol	Joback Method
hf	-49.54	kJ/mol	Joback Method
hfus	17.55	kJ/mol	Joback Method
hvap	43.61	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.695		Crippen Method
mcvol	124.960	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
tb	470.78	K	Joback Method
tc	693.86	K	Joback Method
tf	353.03	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.53	J/mol×K	470.78	Joback Method
cpg	279.65	J/mol×K	507.96	Joback Method
cpg	294.92	J/mol×K	545.14	Joback Method
cpg	309.34	J/mol×K	582.32	Joback Method
cpg	322.95	J/mol×K	619.50	Joback Method
cpg	335.77	J/mol×K	656.68	Joback Method
cpg	347.84	J/mol×K	693.86	Joback Method

Sources

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=R163578&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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