

2-((Z)-2-pentenyl)thiazolidine

Inchi:	InChI=1S/C8H15NS/c1-2-3-4-5-8-9-6-7-10-8/h3-4,8-9H,2,5-7H2,1H3/b4-3-
InchiKey:	SZTKUYBKNVBHRK-ARJAWSKDSA-N
Formula:	C8H15NS
SMILES:	CCC=CCC1NCCS1
Mol. weight [g/mol]:	157.28

Physical Properties

Property code	Value	Unit	Source
gf	260.82	kJ/mol	Joback Method
hf	52.32	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	46.19	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.005		Crippen Method
mcvol	134.750	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinsol	1289.00		NIST Webbook
tb	498.26	K	Joback Method
tc	723.31	K	Joback Method
tf	374.22	K	Joback Method
vc	0.487	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.35	J/mol×K	498.26	Joback Method
cpg	306.63	J/mol×K	535.77	Joback Method
cpg	321.93	J/mol×K	573.28	Joback Method
cpg	336.31	J/mol×K	610.79	Joback Method
cpg	349.81	J/mol×K	648.30	Joback Method
cpg	362.48	J/mol×K	685.81	Joback Method
cpg	374.37	J/mol×K	723.31	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=R163667&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
mccvol:	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

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