Thiazolidine, 2-hexyl-

Other names: 2-Hexylthiazolidine
Inchi: InChI=1S/C9H19NS/c1-2-3-4-5-6-9-10-7-8-11-9/h9-10H,2-8H2,1H3
InchiKey: OAMNFUGALUYNII-UHFFFAOYSA-N
Formula: C9H19NS
SMILES: CCCCCCC1NCCS1
Mol. weight [g/mol]: 173.32
CAS: 40790-77-0

Physical Properties

Property code	Value	Unit	Source
gf	189.02	kJ/mol	Joback Method
hf	-85.54	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	48.45	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.619		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	1402.00		NIST Webbook
rinpol	1402.00		NIST Webbook
tb	516.98	K	Joback Method
tc	728.13	K	Joback Method
tf	390.57	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.60	J/mol×K	516.98	Joback Method
cpg	371.11	J/mol×K	552.17	Joback Method
cpg	387.71	J/mol×K	587.36	Joback Method
cpg	403.43	J/mol×K	622.56	Joback Method
cpg	418.30	J/mol×K	657.75	Joback Method
cpg	432.35	J/mol×K	692.94	Joback Method

cpg	445.61	J/mol×K	728.13	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=C40790770&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