2-octylthiazolidine

Inchi: InChI=1S/C11H23NS/c1-2-3-4-5-6-7-8-11-12-9-10-13-11/h11-12H,2-10H2,1H3
InchiKey: PBDQYMCEPIQARI-UHFFFAOYSA-N
Formula: C11H23NS
SMILES: CCCCCCCCC1NCCS1
Mol. weight [g/mol]: 201.37

Physical Properties

Property code	Value	Unit	Source
gf	205.86	kJ/mol	Joback Method
hf	-126.82	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	52.91	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.399		Crippen Method
mcvol	181.320	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	562.74	K	Joback Method
tc	767.42	K	Joback Method
tf	413.11	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.08	J/mol×K	562.74	Joback Method
cpg	469.92	J/mol×K	596.85	Joback Method
cpg	487.79	J/mol×K	630.97	Joback Method
cpg	504.72	J/mol×K	665.08	Joback Method
cpg	520.74	J/mol×K	699.20	Joback Method
cpg	535.88	J/mol×K	733.31	Joback Method
cpg	550.18	J/mol×K	767.42	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=R163607&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