2-heptylthiazolidine

Other names: Thiazolidine, 2-heptyl-
Inchi: InChI=1S/C10H21NS/c1-2-3-4-5-6-7-10-11-8-9-12-10/h10-11H,2-9H2,1H3
InchiKey: FLUFGKPXTPJANY-UHFFFAOYSA-N
Formula: C10H21NS
SMILES: CCCCCCCC1NCCS1
Mol. weight [g/mol]: 187.34
CAS: 706-19-4

Physical Properties

Property code	Value	Unit	Source
gf	197.44	kJ/mol	Joback Method
hf	-106.18	kJ/mol	Joback Method
hfus	28.84	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.009		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1509.00		NIST Webbook
ripol	2083.00		NIST Webbook
tb	539.86	K	Joback Method
tc	747.72	K	Joback Method
tf	401.84	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.48	J/mol×K	539.86	Joback Method
cpg	419.72	J/mol×K	574.50	Joback Method
cpg	437.01	J/mol×K	609.15	Joback Method
cpg	453.39	J/mol×K	643.79	Joback Method
cpg	468.88	J/mol×K	678.44	Joback Method
cpg	483.52	J/mol×K	713.08	Joback Method

cpg	497.34	J/mol×K	747.72	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=C706194&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume