2-butyl-2-methylthiazolidine

Inchi: InChI=1S/C8H17NS/c1-3-4-5-8(2)9-6-7-10-8/h9H,3-7H2,1-2H3
InchiKey: FRQZYPALTIYXIY-UHFFFAOYSA-N
Formula: C8H17NS
SMILES: CCCCC1(C)NCCS1
Mol. weight [g/mol]: 159.29
CAS: 697-42-7

Physical Properties

Property code	Value	Unit	Source
gf	175.11	kJ/mol	Joback Method
hf	-49.66	kJ/mol	Joback Method
hfus	17.36	kJ/mol	Joback Method
hvap	45.08	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.229		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
ripol	1675.00		NIST Webbook
ripol	1675.00		NIST Webbook
tb	494.34	K	Joback Method
tc	718.22	K	Joback Method
tf	403.20	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.81	J/mol×K	494.34	Joback Method
cpg	324.45	J/mol×K	531.65	Joback Method
cpg	339.99	J/mol×K	568.97	Joback Method
cpg	354.56	J/mol×K	606.28	Joback Method
cpg	368.27	J/mol×K	643.59	Joback Method
cpg	381.25	J/mol×K	680.91	Joback Method
cpg	393.63	J/mol×K	718.22	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=C697427&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume