2-butyl-2-ethylthiazolidine

Inchi: InChI=1S/C9H19NS/c1-3-5-6-9(4-2)10-7-8-11-9/h10H,3-8H2,1-2H3
InchiKey: QQWFGZMIJXDISP-UHFFFAOYSA-N
Formula: C9H19NS
SMILES: CCCCC1(CC)NCCS1
Mol. weight [g/mol]: 173.32

Physical Properties

Property code	Value	Unit	Source
gf	183.53	kJ/mol	Joback Method
hf	-70.30	kJ/mol	Joback Method
hfus	19.95	kJ/mol	Joback Method
hvap	47.30	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.619		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
ripol	1778.00		NIST Webbook
ripol	1778.00		NIST Webbook
tb	517.22	K	Joback Method
tc	737.33	K	Joback Method
tf	414.47	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.47	J/mol×K	517.22	Joback Method
cpg	370.89	J/mol×K	553.90	Joback Method
cpg	387.22	J/mol×K	590.59	Joback Method
cpg	402.59	J/mol×K	627.27	Joback Method
cpg	417.11	J/mol×K	663.96	Joback Method
cpg	430.90	J/mol×K	700.64	Joback Method
cpg	444.10	J/mol×K	737.33	Joback Method

Sources

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=R298892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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