2-ethyl-2-methylthiazolidine

Other names: Thiazolidine, 2-ethyl-2-methyl-
methylethyl thiazolidine
Inchi: InChI=1S/C6H13NS/c1-3-6(2)7-4-5-8-6/h7H,3-5H2,1-2H3
InchiKey: AGSHBVNPPGEAMB-UHFFFAOYSA-N
Formula: C6H13NS
SMILES: CCC1(C)NCCS1
Mol. weight [g/mol]: 131.24
CAS: 694-64-4

Physical Properties

Property code	Value	Unit	Source
gf	158.27	kJ/mol	Joback Method
hf	-8.38	kJ/mol	Joback Method
hfus	12.18	kJ/mol	Joback Method
hvap	40.63	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.449		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	1058.00		NIST Webbook
ripol	1491.00		NIST Webbook
tb	448.58	K	Joback Method
tc	679.92	K	Joback Method
tf	380.66	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.04	J/mol×K	448.58	Joback Method
cpg	236.79	J/mol×K	487.14	Joback Method
cpg	250.42	J/mol×K	525.69	Joback Method
cpg	263.06	J/mol×K	564.25	Joback Method
cpg	274.85	J/mol×K	602.81	Joback Method

cpg	285.91	J/mol×K	641.36	Joback Method
cpg	296.37	J/mol×K	679.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C694644&Units=SI
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

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