2-Methyl-2-hydroxymethylthiazolidine

Inchi: InChI=1S/C5H11NOS/c1-5(4-7)6-2-3-8-5/h6-7H,2-4H2,1H3
InchiKey: INLBSGLZAXEXKR-UHFFFAOYSA-N
Formula: C5H11NOS
SMILES: CC1(CO)NCCS1
Mol. weight [g/mol]: 133.21

Physical Properties

Property code	Value	Unit	Source
gf	13.03	kJ/mol	Joback Method
hf	-139.97	kJ/mol	Joback Method
hfus	13.68	kJ/mol	Joback Method
hvap	55.08	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.031		Crippen Method
mcvol	102.650	ml/mol	McGowan Method
pc	5390.71	kPa	Joback Method
rinpol	1126.00		NIST Webbook
rinpol	1126.00		NIST Webbook
tb	517.88	K	Joback Method
tc	735.93	K	Joback Method
tf	430.21	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.48	J/mol×K	517.88	Joback Method
cpg	239.26	J/mol×K	554.22	Joback Method
cpg	249.29	J/mol×K	590.56	Joback Method
cpg	258.70	J/mol×K	626.90	Joback Method
cpg	267.58	J/mol×K	663.25	Joback Method
cpg	276.05	J/mol×K	699.59	Joback Method
cpg	284.21	J/mol×K	735.93	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=R556980&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume