2-acetyl-2-methylthiazolidine

Inchi: InChI=1S/C6H11NOS/c1-5(8)6(2)7-3-4-9-6/h7H,3-4H2,1-2H3
InchiKey: WLXIBDDBHZVOIL-UHFFFAOYSA-N
Formula: C6H11NOS
SMILES: CC(=O)C1(C)NCCS1
Mol. weight [g/mol]: 145.22

Physical Properties

Property code	Value	Unit	Source
gf	29.35	kJ/mol	Joback Method
hf	-120.96	kJ/mol	Joback Method
hfus	13.78	kJ/mol	Joback Method
hvap	47.37	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	0.628		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1155.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1789.00		NIST Webbook
tb	502.45	K	Joback Method
tc	744.89	K	Joback Method
tf	430.59	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.19	J/mol×K	502.45	Joback Method
cpg	252.38	J/mol×K	542.86	Joback Method
cpg	264.57	J/mol×K	583.26	Joback Method

cpg	275.89	J/mol×K	623.67	Joback Method
cpg	286.50	J/mol×K	664.08	Joback Method
cpg	296.53	J/mol×K	704.49	Joback Method
cpg	306.13	J/mol×K	744.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R187712&Units=SI

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