2-Thiazolidinecarboxamide, 2-methyl-

Other names: 2-Methyl-2-acetamidotetrahydrothiazole
Inchi: InChI=1S/C5H10N2OS/c1-5(4(6)8)7-2-3-9-5/h7H,2-3H2,1H3,(H2,6,8)
InchiKey: JMAFWCZDYHKNPQ-UHFFFAOYSA-N
Formula: C5H10N2OS
SMILES: CC1(C(N)=O)NCCS1
Mol. weight [g/mol]: 146.21
CAS: 13084-22-5

Physical Properties

Property code	Value	Unit	Source
gf	87.38	kJ/mol	Joback Method
hf	-66.53	kJ/mol	Joback Method
hfus	16.39	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-0.70		Crippen Method
logp	-0.476		Crippen Method
mcvol	108.330	ml/mol	McGowan Method
pc	5619.38	kPa	Joback Method
tb	552.10	K	Joback Method
tc	809.39	K	Joback Method
tf	502.58	K	Joback Method
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.57	J/mol×K	552.10	Joback Method
cpg	259.33	J/mol×K	594.98	Joback Method
cpg	270.21	J/mol×K	637.86	Joback Method
cpg	280.36	J/mol×K	680.75	Joback Method
cpg	289.97	J/mol×K	723.63	Joback Method
cpg	299.21	J/mol×K	766.51	Joback Method
cpg	308.25	J/mol×K	809.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13084225&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume